

WEST Search History

DATE: Monday, June 14, 2004

Hide?	Set Name	Query	Hit Count
		<i>DB=PGPB; THES=ASSIGNEE; PLUR=YES; OP=ADJ</i>	
<input type="checkbox"/>	L10	phosphatase adj10 nucleoside	85
		<i>DB=USPT,USOC,EPAB,JPAB,DWPI; THES=ASSIGNEE; PLUR=YES; OP=ADJ</i>	
<input type="checkbox"/>	L9	L8 and muta\$6	75
<input type="checkbox"/>	L8	phosphatase adj10 nucleoside	166
<input type="checkbox"/>	L7	phosphatase adj20 nucleoside	185
<input type="checkbox"/>	L6	phosphatase same nucleoside	518
<input type="checkbox"/>	L5	phosphatase and nucleoside	3980
<input type="checkbox"/>	L4	phosphatase and blattae and nucleoside	4
		<i>DB=PGPB; THES=ASSIGNEE; PLUR=YES; OP=ADJ</i>	
<input type="checkbox"/>	L3	phosphatase and blattae and nucleoside	4
<input type="checkbox"/>	L2	phosphatase same blattae same nucleoside	1
		<i>DB=USPT,USOC,EPAB,JPAB,DWPI; THES=ASSIGNEE; PLUR=YES; OP=ADJ</i>	
<input type="checkbox"/>	L1	phosphatase same blattae same nucleoside	4

END OF SEARCH HISTORY

Hit List

[Clear](#) [Generate Collection](#) [Print](#) [Fwd Refs](#) [Bkwd Refs](#)
[Generate OACS](#)

Search Results - Record(s) 1 through 4 of 4 returned.

☐ 1. Document ID: US 20030215464 A1

L3: Entry 1 of 4

File: PGPB

Nov 20, 2003

PGPUB-DOCUMENT-NUMBER: 20030215464
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20030215464 A1

TITLE: Methods and compositions for vaccination against or involving
enterobacteriaceae bacteria

PUBLICATION-DATE: November 20, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY	RULE-47
Klimpel, Gary R.	Santa Fe	TX	US	
Niesel, David W.	Friendswood	TX	US	
Chopra, Ashok	League City	TX	US	
Sha, Jian	League City	TX	US	

US-CL-CURRENT: [424/200.1](#); [435/252.3](#), [435/252.33](#)

Full	Title	Citation	Front	Review	Classification	Date	Reference	Sequences	Attachments	Claims	KIMC	Draw D
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☐ 2. Document ID: US 20030022163 A1

L3: Entry 2 of 4

File: PGPB

Jan 30, 2003

PGPUB-DOCUMENT-NUMBER: 20030022163
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20030022163 A1

TITLE: Detection of repeated nucleic acid sequences

PUBLICATION-DATE: January 30, 2003

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY	RULE-47
Mandrekar, Michelle N.	Oregon	WI	US	
Tereba, Allan	Fitchburg	WI	US	
Shultz, John William	Verona	WI	US	

US-CL-CURRENT: 435/6; 536/24.3

Full	Title	Citation	Front	Review	Classification	Date	Reference	Sequences	Attachments	Claims	KMC	Draw De
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☐ 3. Document ID: US 20020155556 A1

L3: Entry 3 of 4

File: PGPB

Oct 24, 2002

PGPUB-DOCUMENT-NUMBER: 20020155556
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20020155556 A1

TITLE: Method of producing target substance by fermentation

PUBLICATION-DATE: October 24, 2002

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY	RULE-47
Imaizumi, Akira	Kawasaki-shi		JP	
Usuda, Yoshihiro	Kawasaki-shi		JP	
Sugimoto, Shinichi	Kawasaki-shi		JP	

US-CL-CURRENT: 435/115; 435/252.33, 435/69.1

Full	Title	Citation	Front	Review	Classification	Date	Reference	Sequences	Attachments	Claims	KMC	Draw De
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☐ 4. Document ID: US 20020004590 A1

L3: Entry 4 of 4

File: PGPB

Jan 10, 2002

PGPUB-DOCUMENT-NUMBER: 20020004590
PGPUB-FILING-TYPE: new
DOCUMENT-IDENTIFIER: US 20020004590 A1

TITLE: Method for producing nucleoside-5'-phosphate ester

PUBLICATION-DATE: January 10, 2002

INVENTOR-INFORMATION:

NAME	CITY	STATE	COUNTRY	RULE-47
Mihara, Yasuhiro	Kawasaki-shi		JP	
Utagawa, Takashi	Tokyo		JP	
Yamada, Hideaki	Kyoto-shi		JP	
Asano, Yasuhisa	Toyama-ken		JP	

US-CL-CURRENT: 536/23.2; 435/196

Full	Title	Citation	Front	Review	Classification	Date	Reference	Sequences	Attachments	Claims	KMC	Draw De
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Clear	Generate Collection	Print	Fwd Refs	Ekwd Refs	Generate OACS
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Terms	Documents
phosphatase and blattae and nucleoside	4

Display Format:

[Previous Page](#)

[Next Page](#)

[Go to Doc#](#)

Hit List

Clear	Generate Collection	Print	Fwd Refs	Bkwd Refs
Generate OACS				

Search Results - Record(s) 1 through 4 of 4 returned.

☐ 1. Document ID: US 6355472 B2

Using default format because multiple data bases are involved.

L1: Entry 1 of 4

File: USPT

Mar 12, 2002

US-PAT-NO: 6355472

DOCUMENT-IDENTIFIER: US 6355472 B2

TITLE: Method for producing nucleoside-5'-phosphate ester

DATE-ISSUED: March 12, 2002

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Mihara; Yasuhiro	Kawasaki			JP
Utagawa; Takashi	Tokyo			JP
Yamada; Hideaki	Kyoto			JP
Asano; Yasuhisa	Toyama-ken			JP

US-CL-CURRENT: 435/252.33; 435/194, 435/196, 435/320.1, 536/23.1, 536/23.2

Full	Title	Citation	Front	Review	Classification	Date	Reference			Claims	FIGS	Draw Ds
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☐ 2. Document ID: US 6207435 B1

L1: Entry 2 of 4

File: USPT

Mar 27, 2001

US-PAT-NO: 6207435

DOCUMENT-IDENTIFIER: US 6207435 B1

TITLE: Method for producing nucleoside-5'-phosphate ester

DATE-ISSUED: March 27, 2001

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Mihara; Yasuhiro	Kawasaki			JP
Utagawa; Takashi	Tokyo			JP
Yamada; Hideaki	Kyoto			JP
Asano; Yasuhisa	Imizu-gun			JP

US-CL-CURRENT: 435/196; 435/194, 435/195

ABSTRACT:

A method for producing nucleoside-5'-phosphate esters inexpensively and in high yields by phosphorylating a nucleoside with a phosphatate group donor using an acid phosphatase having an increased affinity for the nucleoside and/or an increased temperature stability at a pH of pH 3.0 to 5.5, to produce a nucleoside-5'-phosphate ester. Mutant acid phosphatases having increased affinity for nucleosides and/or an enhanced temperature stability are also provided.

3 Claims, 13 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 10

Full	Title	Citation	Front	Review	Classification	Date	Reference			Claims	EXMC	Draw. De
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☐ 3. Document ID: US 6015697 A

L1: Entry 3 of 4

File: USPT

Jan 18, 2000

US-PAT-NO: 6015697

DOCUMENT-IDENTIFIER: US 6015697 A

TITLE: Method for producing nucleoside-5'-phosphate ester

DATE-ISSUED: January 18, 2000

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Mihara; Yasuhiro	Kawasaki			JP
Utagawa; Takashi	Tokyo			JP
Yamada; Hideaki	Kyoto			JP
Asano; Yasuhisa	Toyama-ken			JP

US-CL-CURRENT: 435/87; 435/194, 435/195, 435/252.3, 435/252.33, 536/23.2

ABSTRACT:

A method for producing nucleoside-5'-phosphate esters inexpensively and in high yields by phosphorylating a nucleoside with a phosphatate group donor using an acid phosphatase having an increased affinity for the nucleoside and/or an increased temperature stability at a pH of pH 3.0 to 5.5, to produce a nucleoside-5'-phosphate ester. Mutant acid phosphatases having increased affinity for nucleosides and/or an enhanced temperature stability are also provided.

14 Claims, 13 Drawing figures
Exemplary Claim Number: 1
Number of Drawing Sheets: 10

Full	Title	Citation	Front	Review	Classification	Date	Reference			Claims	EXMC	Draw. De
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☐ 4. Document ID: US 6010851 A

L1: Entry 4 of 4

File: USPT

Jan 4, 2000

US-PAT-NO: 6010851

DOCUMENT-IDENTIFIER: US 6010851 A

TITLE: Method for producing nucleoside-5'-phosphate ester

DATE-ISSUED: January 4, 2000

INVENTOR-INFORMATION:

NAME	CITY	STATE	ZIP CODE	COUNTRY
Mihara; Yasuhiro	Kawasaki			JP
Utagawa; Takashi	Kawasaki			JP
Yamada; Hideaki	Kyoto			JP
Asano; Yasuhisa	Imizu-gun			JP

US-CL-CURRENT: 435/6; 536/26.6

ABSTRACT:

Nucleoside-5'-phosphate ester is produced inexpensively and efficiently by allowing an acid phosphatase, especially an acid phosphatase having a lowered phosphomonoesterase activity to act under a condition of pH 3.0 to 5.5 on a nucleoside and a phosphate group donor selected from the group consisting of polyphosphoric acid or a salt thereof, phenylphosphoric acid or a salt thereof, and carbamyl phosphate or a salt thereof to produce nucleoside-5'-phosphate ester, and collecting it.

31 Claims, 12 Drawing figures

Exemplary Claim Number: 1

Number of Drawing Sheets: 11

Full	Title	Citation	Front	Review	Classification	Date	Reference			Claims	RM/C	Draw. Ds
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Clear	Generate Collection	Print	Fwd Refs	Bkwd Refs	Generate OACS
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Terms	Documents
phosphatase same blattae same nucleoside	4

Display Format: [Previous Page](#)[Next Page](#)[Go to Doc#](#)

STN SEARCH

09/807,990

6/14/04

=> s blattae and phosphatase and (structure or crystal or x-ray)

L1 4 FILE MEDLINE
L2 6 FILE CAPLUS
L3 4 FILE SCISEARCH
L4 3 FILE LIFESCI
L5 4 FILE BIOSIS
L6 4 FILE EMBASE

TOTAL FOR ALL FILES

L7 25 BLATTAE AND PHOSPHATASE AND (STRUCTURE OR CRYSTAL OR X-RAY)

=> dup rem l7

PROCESSING COMPLETED FOR L7

L8 7 DUP REM L7 (18 DUPLICATES REMOVED)

=> d ibib abs

L8 ANSWER 1 OF 7 MEDLINE on STN
ACCESSION NUMBER: 2004270499 IN-PROCESS
DOCUMENT NUMBER: PubMed ID: 15170108
TITLE: Improving the Pyrophosphate-inosine Phosphotransferase
Activity of Escherichia **blattae** Acid
Phosphatase by Sequential Site-directed
Mutagenesis.
AUTHOR: Mihara Yasuhiro; Ishikawa Kohki; Suzuki Ei-Ichiro; Asano
Yasuhisa
CORPORATE SOURCE: Applied Microbiology Laboratory, Fermentation and
Biotechnology Laboratories, Ajinomoto Co., Inc.
SOURCE: Bioscience, biotechnology, and biochemistry, (2004 May) 68
(5) 1046-50.
Journal code: 9205717. ISSN: 0916-8451.
PUB. COUNTRY: Japan
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: IN-DATA-REVIEW; IN-PROCESS; NONINDEXED; Priority Journals
ENTRY DATE: Entered STN: 20040602
Last Updated on STN: 20040602

AB Escherichia **blattae** acid **phosphatase**
/phosphotransferase (EB-AP/PTase) exhibits C-5'-position selective
pyrophosphate-nucleoside phosphotransferase activity in addition to its
intrinsic **phosphatase**. Improvement of its phosphotransferase
activity was investigated by sequential site-directed mutagenesis. By
comparing the primary **structures** of higher 5'-inosinic acid
(5'-IMP) productivity and lower 5'-IMP productivity acid
phosphatase/phosphotransferase, candidate residues of substitution
were selected. Then a total of 11 amino acid substitutions were made with
sequential substitutions. As the number of substituted amino acid
residues increased, the 5'-IMP productivity of the mutant enzyme
increased, and the activity of the 11 mutant phosphotransferases of
EB-AP/PTase reached the same level as that of *Morganella morganii*
AP/PTase. This result shows that Leu63, Ala65, Glu66, Asn69, Ser71,
Asp116, Thr135, and Glu136, whose relevance was not directly established
by structural analysis alone, also plays an important role in the
phosphotransferase activity of EB-AP/PTase.

L8 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:19321 CAPLUS
DOCUMENT NUMBER: 136:84776
TITLE: Enzymic method of nucleoside-5'-phosphate
INVENTOR(S): Iida, Iwao; Arashida, Takaki; Abe, Shigemitsu
PATENT ASSIGNEE(S): Ajinomoto Co., Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

 JP 2002000289 A2 20020108 JP 2000-189226 20000623
 PRIORITY APPLN. INFO.: JP 2000-189226 20000623
 OTHER SOURCE(S): CASREACT 136:84776

AB Nucleosides, esp. low-soly. nucleosides, or their precursor
crystal is phys. pulverized to a size having sp. surface area of
 0.4 m²/g, incubated with enzyme such as acidic **phosphatase** in
 the presence of an phosphate donor to prep. nucleoside-5'-phosphate.
 Manuf. of 5'-guanylic acid from guanosine **crystal** in the
 presence of pyrophosphoric acid with acidic **phosphatase** mutant
 of Escherichia **blattae** was shown.

L8 ANSWER 3 OF 7 MEDLINE on STN DUPLICATE 1
 ACCESSION NUMBER: 2002471678 MEDLINE
 DOCUMENT NUMBER: PubMed ID: 12200535
 TITLE: Enhancement of nucleoside phosphorylation activity in an
 acid **phosphatase**.
 AUTHOR: Ishikawa Kohki; Mihara Yasuhiro; Shimba Nobuhisa; Ohtsu
 Naoko; Kawasaki Hisashi; Suzuki Ei-ichiro; Asano Yasuhisa
 CORPORATE SOURCE: Central Research Laboratories, Ajinomoto Co., Inc., 1-1
 Suzuki-cho Kawasaki-ku, Kawasaki 210-868, Japan.
 SOURCE: Protein engineering, (2002 Jul) 15 (7) 539-43.
 Journal code: 8801484. ISSN: 0269-2139.
 PUB. COUNTRY: England: United Kingdom
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals
 ENTRY MONTH: 200302
 ENTRY DATE: Entered STN: 20020918
 Last Updated on STN: 20030212
 Entered Medline: 20030211

AB Escherichia **blattae** non-specific acid **phosphatase**
 (EB-NSAP) possesses a pyrophosphate-nucleoside phosphotransferase
 activity, which is C-5'-position selective. Current mutational and
 structural data were used to generate a mutant EB-NSAP for a potential
 industrial application as an effective and economical protein catalyst in
 synthesizing nucleotides from nucleosides. First, Gly74 and Ile153 were
 replaced by Asp and Thr, respectively, since the corresponding
 replacements in the homologous enzyme from Morganella morganii reduced the
 K(m) value for inosine and thus increased the productivity of 5'-IMP. We
 determined the **crystal structure** of G74D/I153T, which
 has a reduced K(m) value for inosine, as expected. The tertiary
structure of G74D/I153T was virtually identical to that of the
 wild-type. In addition, neither of the introduced side chains of Asp74
 and Thr153 is directly involved in the interaction with inosine in a
 hypothetical binding mode of inosine to EB-NSAP, although both residues
 are situated near a potential inosine-binding site. These findings
 suggested that a slight structural change caused by an amino acid
 replacement around the potential inosine-binding site could significantly
 reduce the K(m) value. Prompted by this hypothesis, we designed several
 mutations and introduced them to G74D/I153T, to decrease the K(m) value
 further. This strategy produced a S72F/G74D/I153T mutant with a 5.4-fold
 lower K(m) value and a 2.7-fold higher V(max) value as compared to the
 wild-type EB-NSAP.

L8 ANSWER 4 OF 7 MEDLINE on STN DUPLICATE 2
 ACCESSION NUMBER: 2002117993 MEDLINE
 DOCUMENT NUMBER: PubMed ID: 11852042
 TITLE: Shigella apyrase--a novel variant of bacterial acid
 phosphatases?
 AUTHOR: Babu M Madan; Kamalakkannan S; Subrahmanyam Yerramalli V B
 K; Sankaran Krishnan
 CORPORATE SOURCE: Centre for Biotechnology, Anna University, 600 025,
 Chennai, India.
 SOURCE: FEBS letters, (2002 Feb 13) 512 (1-3) 8-12.
 Journal code: 0155157. ISSN: 0014-5793.
 PUB. COUNTRY: Netherlands
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals
 ENTRY MONTH: 200203

ENTRY DATE: Entered STN: 20020220
 Last Updated on STN: 20020403
 Entered Medline: 20020328

AB A virulence-associated ATP diphosphohydrolase activity in the periplasm of Shigella, identified as apyrase, was found to be markedly similar to bacterial non-specific acid **phosphatases** in primary **structure**. When the Shigella apyrase sequence was threaded in to the recently published 3D **structure** of the highly similar (73%) Escherichia **blattae** acid **phosphatase** it was found to have a highly overlapping 3D **structure**. Our analysis, which included assays for **phosphatase**, haloperoxidase and catalase activities, led us to hypothesize that Shigella apyrase might belong to a new class of pyrophosphatase originating as one more variant in the family of bacterial non-specific acid **phosphatases**. It revealed interesting **structure**-function relationships and probable roles relevant to pathogenesis.

L8 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:185898 CAPLUS
 DOCUMENT NUMBER: 134:233616
 TITLE: Nucleoside-5'-phosphate producing enzyme mutants with enhanced activity designed from **x-ray crystal structure** analysis

INVENTOR(S): Ishikawa, Kohki; Suzuki, Ei-ichiro; Gondoh, Keiko; Shimba, Nobuhisa; Mihara, Yasuhiro; Kawasaki, Hisashi; Kurahashi, Osamu; Kouda, Tohru; Shimaoka, Megumi; Kozutsumi, Rie; Asano, Yasuhisa

PATENT ASSIGNEE(S): Ajinomoto Co., Inc., Japan
 SOURCE: PCT Int. Appl., 150 pp.
 CODEN: PIXXD2

DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001018184	A1	20010315	WO 2000-JP5973	20000901
W:		AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM		
RW:		GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG		
JP 2001136984	A2	20010522	JP 2000-262120	20000831
BR 2000007056	A	20010814	BR 2000-7056	20000901
PRIORITY APPLN. INFO.:			JP 1999-249545	A 19990903
			WO 2000-JP5973	W 20000901

AB A variant nucleoside-5'-phosphate producing enzymes (nucleoside-5'-phosphate synthase) having an elevated nucleoside-5'-phosphate prodn. activity, phosphotransferase activity and/or **phosphatase** activity, are disclosed. By identifying variations on the basis of **x-ray** structural anal. of known enzyme **crystals**, it is found out that the above enzyme has a **structure** wherein, in the nucleoside-5'-phosphate producing enzyme, a Lys residue, two Arg residues and two His residues are present, the C.alpha. distances among these residues fall within a specific range, and there is a space allowing the attachment of nucleoside around these residues. Acid **phosphatase** (AP) from Escherichia **blattae**, other Escherichia species, Morganella, Providencia, Enterobacter, or Klebsiella, can be used for **x-ray crystal structure** anal. Prepn. of nucleotidase activity acid **phosphatase** mutants of Escherichia **blattae** strain JCM1650, Morganella morganii, and Enterobacter aerogenes by substitution at Gly74Asp, Ile153Thr, or at other defined positions such as Ser72, was shown. Enhanced 5'-inosinic acid prodn. and phosphate transfer activity, accompanies by lower Km values for inosine, and compared with that of

wild-type and the mutant enzymes was also demonstrated. At. coordinates
data from the **X-ray crystal**
structure of AP complexed with molybdic acid (molybdate) was used
for anal. and design. A process for efficiently and economically
producing a nucleoside-5'-phosphate using the mutant enzyme is claimed.
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 3
ACCESSION NUMBER: 2001:691370 CAPLUS
DOCUMENT NUMBER: 135:354519
TITLE: Acid **phosphatase**/phosphotransferases from
enteric bacteria
AUTHOR(S): Mihara, Yasuhiro; Utagawa, Takashi; Yamada, Hideaki;
Asano, Yasuhisa
CORPORATE SOURCE: Applied Microbiology Laboratory, Fermentation and
Biotechnology Laboratories, Ajinomoto Co., Inc.,
Kawasaki, 210-8681, Japan
SOURCE: Journal of Bioscience and Bioengineering (2001),
92(1), 50-54
CODEN: JBBIF6; ISSN: 1389-1723
PUBLISHER: Society for Bioscience and Bioengineering, Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We have investigated the enzymic phosphorylation of nucleosides and found
that *Morganella morganii* phoC acid **phosphatase** exhibits
regioselective pyrophosphate (PPi)-nucleoside phosphotransferase activity.
In this study, we isolated genes encoding an acid **phosphatase**
with regioselective phosphotransferase activity (AP/PTase) from
Providencia stuartii, *Enterobacter aerogenes*, *Escherichia blattae*
and *Klebsiella planticola*, and compared the primary **structures**
and enzymic characteristics of these enzymes with those of AP/PTase (PhoC
acid **phosphatase**) from *M. morganii*. The enzymes were highly
homologous in primary **structure** with *M. morganii* AP/PTase, and
are classified as class A1 acid **phosphatases**. The synthesis of
inosine-5'-monophosphate (5'-IMP) by *E. coli* over-producing each acid
phosphatase was investigated. The *P. stuartii* enzyme, which is
most closely related to the *M. morganii* enzyme, exhibited high 5'-IMP
productivity, similar to the *M. morganii* enzyme. The 5'-IMP
productivities of the *E. aerogenes*, *E. blattae* and *K. planticola*
enzymes were inferior to those of the former two enzymes. This result
underlines the importance of lower Km values for efficient nucleotide
prodn. As these enzymes exhibited a very high degree of homol. at the
amino acid sequence level, it is likely that local sequence differences in
the binding pocket are responsible for the differences in the
nucleoside-PPi phosphotransferase reaction.
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 7 OF 7 MEDLINE on STN DUPLICATE 4
ACCESSION NUMBER: 2000296667 MEDLINE
DOCUMENT NUMBER: PubMed ID: 10835340
TITLE: **X-ray structures** of a novel
acid **phosphatase** from *Escherichia blattae*
and its complex with the transition-state analog molybdate.
AUTHOR: Ishikawa K; Mihara Y; Gondoh K; Suzuki E; Asano Y
CORPORATE SOURCE: Central Research Laboratories, Ajinomoto Co., Inc., 1-1
Suzuki-cho, Kawasaki-ku, Kawasaki 210-8681, Japan.
SOURCE: EMBO journal, (2000 Jun 1) 19 (11) 2412-23.
Journal code: 8208664. ISSN: 0261-4189.
PUB. COUNTRY: ENGLAND: United Kingdom
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200007
ENTRY DATE: Entered STN: 20000728
Last Updated on STN: 20000728
Entered Medline: 20000720
AB The **structure** of *Escherichia blattae* non-specific acid
phosphatase (EB-NSAP) has been determined at 1.9 Å resolution with
a bound sulfate marking the phosphate-binding site. The enzyme is a 150

kDa homohehexamer. EB-NSAP shares a conserved sequence motif not only with several lipid **phosphatases** and the mammalian glucose-6-**phosphatases**, but also with the vanadium-containing chloroperoxidase (CPO) of *Curvularia inaequalis*. Comparison of the **crystal structures** of EB-NSAP and CPO reveals striking similarity in the active site **structures**. In addition, the topology of the EB-NSAP core shows considerable similarity to the fold of the active site containing part of the monomeric 67 kDa CPO, despite the lack of further sequence identity. These two enzymes are apparently related by divergent evolution. We have also determined the **crystal structure** of EB-NSAP complexed with the transition-state analog molybdate. Structural comparison of the native enzyme and the enzyme-molybdate complex reveals that the side-chain of His150, a putative catalytic residue, moves toward the molybdate so that it forms a hydrogen bond with the metal oxyanion when the molybdenum forms a covalent bond with NE2 of His189.

```
=> s (phosphatase or kinase or phosphotransferase) and nucleoside-5(1w)-phosphate and muta?
TOTAL FOR ALL FILES
L15          6 (PHOSPHATASE OR KINASE OR PHOSPHOTRANSFERASE) AND NUCLEOSIDE-5(1
L16          W) -PHOSPHATE AND MUTA?
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=> dup rem l15
PROCESSING COMPLETED FOR L15
L16          6 DUP REM L15 (0 DUPLICATES REMOVED)
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=> d ibib abs 1-6
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```
L16 ANSWER 1 OF 6  CAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:    2002:19321  CAPLUS
DOCUMENT NUMBER:     136:84776
TITLE:               Enzymic method of nucleoside-5'-phosphate
INVENTOR(S):         Iida, Iwao; Arashida, Takaki; Abe, Shigemitsu
PATENT ASSIGNEE(S):  Ajinomoto Co., Inc., Japan
SOURCE:              Jpn. Kokai Tokkyo Koho, 10 pp.
                     CODEN: JKXXAF
DOCUMENT TYPE:        Patent
LANGUAGE:             Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:
```

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002000289	A2	20020108	JP 2000-189226	20000623
PRIORITY APPLN. INFO.:			JP 2000-189226	20000623

```
OTHER SOURCE(S):      CASREACT 136:84776
AB  Nucleosides, esp. low-soly. nucleosides, or their precursor crystal is
phys. pulverized to a size having sp. surface area of 0.4 m2/g, incubated
with enzyme such as acidic phosphatase in the presence of an
phosphate donor to prep. nucleoside-5'-phosphate. Manuf. of 5'-guanylic acid from guanosine crystal in
the presence of pyrophosphoric acid with acidic phosphatase
mutant of Escherichia blattae was shown.
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L16 ANSWER 2 OF 6  BIOSIS  COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
ACCESSION NUMBER:    2002:278589  BIOSIS
DOCUMENT NUMBER:     PREV200200278589
TITLE:               Method for producing nucleoside-5'-phosphate ester.
AUTHOR(S):           Mihara, Yasuhiro [Inventor, Reprint author]; Utagawa,
                     Takashi [Inventor]; Yamada, Hideaki [Inventor]; Asano,
                     Yasuhisa [Inventor]
CORPORATE SOURCE:     Kawasaki, Japan
ASSIGNEE:             Ajinomoto Co., Inc., Tokyo, Japan
PATENT INFORMATION:   US 6355472 March 12, 2002
SOURCE:              Official Gazette of the United States Patent and Trademark
                     Office Patents, (Mar. 12, 2002) Vol. 1256, No. 2.
                     http://www.uspto.gov/web/menu/patdata.html. e-file.
                     CODEN: OGUPE7. ISSN: 0098-1133.
DOCUMENT TYPE:        Patent
```

LANGUAGE: English
ENTRY DATE: Entered STN: 8 May 2002
Last Updated on STN: 8 May 2002

AB A method for producing **nucleoside-5'-phosphate** esters inexpensively and in high yields by phosphorylating a nucleoside with a phosphate group donor using an acid **phosphatase** having an increased affinity for the nucleoside and/or an increased temperature stability at a pH of pH 3.0 to 5.5, to produce a **nucleoside-5'-phosphate** ester. **Mutant** acid **phosphatases** having increased affinity for nucleosides and/or an enhanced temperature stability are also provided.

L16 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:185898 CAPLUS

DOCUMENT NUMBER: 134:233616

TITLE: **Nucleoside-5'-phosphate**
producing enzyme **mutants** with enhanced activity designed from x-ray crystal structure analysis

INVENTOR(S): Ishikawa, Kohki; Suzuki, Ei-ichiro; Gondoh, Keiko; Shimba, Nobuhisa; Mihara, Yasuhiro; Kawasaki, Hisashi; Kurahashi, Osamu; Kouda, Tohru; Shimaoka, Megumi; Kozutsumi, Rie; Asano, Yasuhisa

PATENT ASSIGNEE(S): Ajinomoto Co., Inc., Japan

SOURCE: PCT Int. Appl., 150 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001018184	A1	20010315	WO 2000-JP5973	20000901
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
JP 2001136984	A2	20010522	JP 2000-262120	20000831
BR 2000007056	A	20010814	BR 2000-7056	20000901
PRIORITY APPLN. INFO.:			JP 1999-249545	A 19990903
			WO 2000-JP5973	W 20000901

AB A variant **nucleoside-5'-phosphate** producing enzymes (**nucleoside-5'-phosphate** synthase) having an elevated **nucleoside-5'-phosphate** prodn. activity, **phosphotransferase** activity and/or **phosphatase** activity, are disclosed. By identifying variations on the basis of x-ray structural anal. of known enzyme crystals, it is found out that the above enzyme has a structure wherein, in the **nucleoside-5'-phosphate** producing enzyme, a Lys residue, two Arg residues and two His residues are present, the C.alpha. distances among these residues fall within a specific range, and there is a space allowing the attachment of nucleoside around these residues. Acid **phosphatase** (AP) from *Escherichia blattae*, other *Escherichia* species, *Morganella*, *Providencia*, *Enterobacter*, or *Klebsiella*, can be used for x-ray crystal structure anal. Prepn. of nucleotidase activity acid **phosphatase mutants** of *Escherichia blattae* strain JCM1650, *Morganella morganii*, and *Enterobacter aerogenes* by substitution at Gly74Asp, Ile153Thr, or at other defined positions such as Ser72, was shown. Enhanced 5'-inosinic acid prodn. and phosphate transfer activity, accompanies by lower Km values for inosine, and compared with that of wild-type and the **mutant** enzymes was also demonstrated. At. coordinates data from the X-ray crystal structure of AP complexed with molybdic acid (molybdate) was used for anal. and design. A process for efficiently and economically producing a **nucleoside-5'-phosphate** using the **mutant** enzyme is claimed.

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 4 OF 6 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
ACCESSION NUMBER: 2001:440002 BIOSIS
DOCUMENT NUMBER: PREV200100440002
TITLE: Method for producing **nucleoside-5'-phosphate** ester.
AUTHOR(S): Mihara, Yasuhiro [Inventor, Reprint author]; Utagawa, Takashi [Inventor]; Yamada, Hideaki [Inventor]; Asano, Yasuhisa [Inventor]
CORPORATE SOURCE: Kawasaki, Japan
ASSIGNEE: Ajinomoto Co., Inc., Tokyo, Japan
PATENT INFORMATION: US 6207435 March 27, 2001
SOURCE: Official Gazette of the United States Patent and Trademark Office Patents, (Mar. 27, 2001) Vol. 1244, No. 4. e-file. CODEN: OGUPE7. ISSN: 0098-1133.
DOCUMENT TYPE: Patent
LANGUAGE: English
ENTRY DATE: Entered STN: 19 Sep 2001
Last Updated on STN: 22 Feb 2002

AB A method for producing **nucleoside-5'-phosphate** esters inexpensively and in high yields by phosphorylating a nucleoside with a phosphatase group donor using an acid **phosphatase** having an increased affinity for the nucleoside and/or an increased temperature stability at a pH of pH 3.0 to 5.5, to produce a **nucleoside-5'-phosphate** ester. **Mutant** acid **phosphatases** having increased affinity for nucleosides and/or an enhanced temperature stability are also provided.

L16 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:504855 CAPLUS
DOCUMENT NUMBER: 129:186140
TITLE: **Nucleoside-5'-phosphate** and its enzymic production with microbial acid **phosphatase** and **mutants**
INVENTOR(S): Mihara, Yasuhiro; Utagawa, Takashi; Yamada, Hideaki; Asano, Yasuhisa
PATENT ASSIGNEE(S): Ajinomoto Co., Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 44 pp. CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10201481	A2	19980804	JP 1997-161674	19970618
EP 857788	A2	19980812	EP 1997-309365	19971120
EP 857788	A3	19991215		
EP 857788	B1	20030423		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
ES 2199330	T3	20040216	ES 1997-309365	19971120
CN 1184157	A	19980610	CN 1997-122934	19971121
CN 1117870	B	20030813		
BR 9705813	A	19990427	BR 1997-5813	19971121
US 6015697	A	20000118	US 1997-975698	19971121
US 6207435	B1	20010327	US 1999-417090	19991013
US 2002004590	A1	20020110	US 2000-727578	20001204
US 6355472	B2	20020312		
PRIORITY APPLN. INFO.:			JP 1996-311103	A 19961121
			JP 1997-161674	A 19970618
			US 1997-975698	A3 19971121
			US 1999-417090	A3 19991013

AB Disclosed is a method for efficiently producing **nucleoside-5'-phosphates**, which method comprises treating a nucleoside and a phosphoric acid donor at pH 3.0-5.5, with an acidic **phosphatase** or **mutants** with improved substrate affinity (Km <100) and stability. The enzyme has been produced from *Morganella*

morganii, Escherichia blattae, Providencia stuartii, Enterobacter aerogenes, Klebsiella planticola, and Serratia ficaria, and their encoding DNA are isolated. Prepn. of nucleotidase activity-low acidic **phosphatase mutants** of Escherichia blattae strain JCM1650 by substitution at 74-Gly.fwdarw.Asp, 153-Ile.fwdarw.Thr, 74-Gly.fwdarw.Asp and 153-Ile.fwdarw.Thr, or at other defined positions was shown. Prodn. of 5'-inosinic acid, 5'-guanylic acid, 5'-uridylic acid, and 5'-cytidylic acid with the wild-type and the **mutant** enzymes was also demonstrated.

L16 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1997:61305 CAPLUS

DOCUMENT NUMBER: 126:72040

TITLE: **Nucleoside-5'-phosphate**
and its enzymic production with microbial acid
phosphatase

INVENTOR(S): Mihara, Yasuhiro; Utagawa, Takashi; Yamada, Hideaki;
Asano, Yasuhisa

PATENT ASSIGNEE(S): Ajinomoto Co., Inc., Japan

SOURCE: PCT Int. Appl., 94 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9637603	A1	19961128	WO 1996-JP1402	19960524
W: BR, CA, CN, HU, JP, KR, PL, US, VN				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 09037785	A2	19970210	JP 1996-94680	19960326
CA 2221774	AA	19961128	CA 1996-2221774	19960524
EP 832970	A1	19980401	EP 1996-914437	19960524
R: CH, DE, ES, FR, GB, IT, LI, NL				
CN 1191566	A	19980826	CN 1996-195770	19960524
CN 1105778	B	20030416		
JP 3180349	B2	20010625	JP 1996-535568	19960524
JP 2001245676	A2	20010911	JP 2000-395323	19960524
PL 183293	B1	20020628	PL 1996-323493	19960524
US 6010851	A	20000104	US 1997-750145	19970121
PRIORITY APPLN. INFO.:			JP 1995-149781	A 19950525
			JP 1996-94680	A 19960326
			JP 1996-535568	A3 19960524
			WO 1996-JP1402	W 19960524

AB A process for efficiently and economically producing a **nucleoside -5'-phosphate** which comprises treating a nucleoside and a phosphoric acid donor selected from the group consisting of poly-phosphoric acid (salts), phenylphosphoric acid (salts) and carbamyl phosphoric acid (salts) with an acid **phosphatase**, in particular the one having lowered nucleotidase activity, at pH 3.0.apprx.5.5. The enzyme has been produced from Morganella morganii, Escherichia blattae, Providencia stuartii, Enterobacter aerogenes, Klebsiella planticola, and Serratia ficaria, and their encoding DNA are isolated. The **mutants** of the enzyme with lowered nucleotidase activity can be obtained by site-specific **mutation** at, e.g., 72-Gly and/or 151-Ile of that of Morganella morganii. Prodn. of 5'-inosinic acid, 5'-guanylic acid, 5'-uridylic acid, and 5'-cytidylic acid without nucleoside-2'-ester and nucleoside-3'-ester byproducts was shown.

=> s phosphatase and (crystal or x-ray or three (1w) dimension)

TOTAL FOR ALL FILES

L23 10936 PHOSPHATASE AND (CRYSTAL OR X-RAY OR THREE (1W) DIMENSION)

=> s l23 and acid phosphatase

TOTAL FOR ALL FILES

L30 1966 L23 AND ACID PHOSPHATASE

=> s l30 and bacteria?

TOTAL FOR ALL FILES

L37 84 L30 AND BACTERIA?

=> dup rem 137
PROCESSING COMPLETED FOR L37
L38 49 DUP REM L37 (35 DUPLICATES REMOVED)

=> d ibib abs 1-49

L38 ANSWER 1 OF 49 SCISEARCH COPYRIGHT 2004 THOMSON ISI on STN
ACCESSION NUMBER: 2004:57067 SCISEARCH
THE GENUINE ARTICLE: 759DJ
TITLE: Metal binding Asp-120 in metallo-beta-lactamase L1 from
Stenotrophomonas maltophilia plays a crucial role in
catalysis
AUTHOR: Garrity J D; Carenbauer A L; Herron L R; Crowder M W
(Reprint)
CORPORATE SOURCE: Miami Univ, Dept Chem & Biochem, 112 Hughes Hall, Oxford,
OH 45056 USA (Reprint); Miami Univ, Dept Chem & Biochem,
Oxford, OH 45056 USA
COUNTRY OF AUTHOR: USA
SOURCE: JOURNAL OF BIOLOGICAL CHEMISTRY, (9 JAN 2004) Vol. 279,
No. 2, pp. 920-927.
Publisher: AMER SOC BIOCHEMISTRY MOLECULAR BIOLOGY INC,
9650 ROCKVILLE PIKE, BETHESDA, MD 20814-3996 USA.
ISSN: 0021-9258.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 70
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS
AB Metallo-beta-lactamase L1 from Stenotrophomonas maltophilia is a
dinuclear Zn(II) enzyme that contains a metal-binding aspartic acid in a
position to potentially play an important role in catalysis. The presence
of this metal-binding aspartic acid appears to be common to most
dinuclear, metal-containing, hydrolytic enzymes; particularly those with a
beta-lactamase fold. In an effort to probe the catalytic and metal-binding
role of Asp-120 in L1, three site-directed mutants (D120C, D120N, and
D120S) were prepared and characterized using metal analyses, circular
dichroism spectroscopy, and pre-steady-state and steady-state kinetics.
The D120C, D120N, and D120S mutants were shown to bind 1.6+/-0.2,
1.8+/-0.2, and 1.1+/-0.2 mol of Zn(II) per monomer, respectively. The
mutants exhibited 10- to 1000-fold drops in k(cat) values as compared with
wild-type L1, and a general trend of activity, wild-type>D120N>D120C and
D120S, was observed for all substrates tested. Solvent isotope and pH
dependence studies indicate one or more protons in flight, with pK(a)
values outside the range of pH 5-10 (except D120N), during a rate-limiting
step for all the enzymes. These data demonstrate that Asp-120 is crucial
for L1 to bind its full complement of Zn(II) and subsequently for proper
substrate binding to the enzyme. This work also confirms that Asp-120
plays a significant role in catalysis, presumably via hydrogen bonding
with water, assisting in formation of the bridging hydroxide/water, and a
rate-limiting proton transfer in the hydrolysis reaction.

L38 ANSWER 2 OF 49 MEDLINE on STN DUPLICATE 1
ACCESSION NUMBER: 2003606063 MEDLINE
DOCUMENT NUMBER: PubMed ID: 14687572
TITLE: The first structure of a **bacterial** class B
Acid phosphatase reveals further
structural heterogeneity among **phosphatases** of
the haloacid dehalogenase fold.
AUTHOR: Calderone Vito; Forleo Costantino; Benvenuti Manuela;
Cristina Thaller Maria; Maria Rossolini Gian; Mangani
Stefano
CORPORATE SOURCE: Dipartimento di Chimica, Universita di Siena, Via Aldo
Moro, I-53100 Siena, Italy.
SOURCE: Journal of molecular biology, (2004 Jan 16) 335 (3) 761-73.
Journal code: 2985088R. ISSN: 0022-2836.
PUB. COUNTRY: England: United Kingdom
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200402
ENTRY DATE: Entered STN: 20031223

Last Updated on STN: 20040204
Entered Medline: 20040203

AB AphA is a periplasmic **acid phosphatase** of *Escherichia coli* belonging to class B **bacterial phosphatases**, which is part of the DDDD superfamily of phosphohydrolases. The **crystal** structure of AphA has been determined at 2.2Å and its resolution extended to 1.7Å on an AuCl₃ derivative. This represents the first **crystal** structure of a class B **bacterial phosphatase**. Despite the lack of sequence homology, the AphA structure reveals a haloacid dehalogenase-like fold. This finding suggests that this fold could be conserved among members of the DDDD superfamily of phosphohydrolases. The active enzyme is a homotetramer built by using an extended N-terminal arm intertwining the four monomers. The active site of the native enzyme, as prepared, hosts a magnesium ion, which can be replaced by other metal ions. The structure explains the non-specific behaviour of AphA towards substrates, while a structure-based alignment with other **phosphatases** provides clues about the catalytic mechanism.

L38 ANSWER 3 OF 49 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
DUPLICATE 2

ACCESSION NUMBER: 2003:466567 BIOSIS
DOCUMENT NUMBER: PREV200300466567
TITLE: Functional insights revealed by the **crystal** structures of *Escherichia coli* glucose-1-**phosphatase**.
AUTHOR(S): Lee, Daniel C.; Cottrill, Michael A.; Forsberg, Cecil W.; Jia, Zongchao [Reprint Author]
CORPORATE SOURCE: Department of Biochemistry, Queen's University, Kingston, ON, K7L 3N6, Canada
jia@post.queensu.ca
SOURCE: Journal of Biological Chemistry, (August 15 2003) Vol. 278, No. 33, pp. 31412-31418. print.
CODEN: JBCHA3. ISSN: 0021-9258.
DOCUMENT TYPE: Article
LANGUAGE: English
ENTRY DATE: Entered STN: 8 Oct 2003
Last Updated on STN: 8 Oct 2003

AB The *Escherichia coli* periplasmic glucose-1-**phosphatase** is a member of the histidine **acid phosphatase** family and acts primarily as a glucose scavenger. Previous substrate profiling studies have demonstrated some of the intriguing properties of the enzyme, including its unique and highly selective inositol **phosphatase** activity. The enzyme is also potentially involved in pathogenic inositol phosphate signal transduction pathways via type III secretion into the host cell. We have determined the **crystal** structure of *E. coli* glucose-1-**phosphatase** in an effort to unveil the structural mechanism underlying such unique substrate specificity. The structure was determined by the method of multiwavelength anomalous dispersion using a tungstate derivative together with the H18A inactive mutant complex structure with glucose 1-phosphate at 2.4-Å resolution. In the active site of glucose-1-**phosphatase**, there are two unique gating residues, Glu-196 and Leu-24, in addition to the conserved features of histidine **acid phosphatases**. Together they create steric and electrostatic constraints responsible for the unique selectivity of the enzyme toward phytate and glucose-1-phosphate as well as its unusually high pH optimum for the latter. Based on the structural characterization, we were able to derive simple structural principles that not only precisely explains the substrate specificity of glucose-1-**phosphatase** and the hydrolysis products of various inositol phosphate substrates but also rationalizes similar general characteristics across the histidine **acid phosphatase** family.

L38 ANSWER 4 OF 49 SCISEARCH COPYRIGHT 2004 THOMSON ISI on STN

ACCESSION NUMBER: 2003:377267 SCISEARCH
THE GENUINE ARTICLE: 670JV
TITLE: An iron-dependent **bacterial** phospholipase D reminiscent of purple **acid phosphatases**
AUTHOR: Zambonelli C; Roberts M F (Reprint)
CORPORATE SOURCE: Boston Coll, Merkert Chem Ctr, 2609 Beacon St, Chestnut Hill, MA 02467 USA (Reprint); Boston Coll, Merkert Chem

Ctr, Chestnut Hill, MA 02467 USA
COUNTRY OF AUTHOR: USA
SOURCE: JOURNAL OF BIOLOGICAL CHEMISTRY, (18 APR 2003) Vol. 278,
No. 16, pp. 13706-13711.
Publisher: AMER SOC BIOCHEMISTRY MOLECULAR BIOLOGY INC,
9650 ROCKVILLE PIKE, BETHESDA, MD 20814-3996 USA.
ISSN: 0021-9258.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 44

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB Recombinant phospholipase D (PLD) from *Streptomyces chromofuscus* (scPLD) has been characterized using colorimetric assays, spectroscopic investigations, and site-directed mutagenesis. scPLD, which shows phosphodiesterase activity toward a wide variety of phospholipids and **phosphatase** activity toward p-nitrophenyl phosphate, exhibits a visible absorption band with A-a. at 570 nm. Metal ion analysis performed by inductively coupled plasma mass spectroscopy shows the presence of similar to equivalent of iron, 0.27 equivalent of manganese, and 0.1 equivalent of zinc per mole of protein as isolated. The metal ion content coupled with the visible absorption feature is compatible with the presence of Fe³⁺-tyrosinate coordination. When scPLD was dialyzed against solutions containing Mn²⁺, Zn²⁺ or EDTA, the Fe³⁺ content was reduced to variable extents, and the residual specific activity correlated well with the residual iron content. Sequence homology with metal ion binding motifs in known alkaline **phosphatases** and purple **acid phosphatase** from red kidney bean shows that most of the residues involved in metal ion coordination are conserved among all the sequences considered. Mutation of some of these conserved residues (C123A, D151A, Y154F, and H391A) produced enzymes lacking iron with dramatically reduced PLD activity but little change in secondary structure or ability to bind to small unilamellar vesicles of phosphatidylcholine (with Ba²⁺) or phosphatidic acid. We suggest that scPLD is a member of a family of phosphodiesterase/**phosphatases** with structural and mechanistic similarity to iron-dependent purple **acid phosphatases**.

L38 ANSWER 5 OF 49 MEDLINE on STN
ACCESSION NUMBER: 2004139561 MEDLINE
DOCUMENT NUMBER: PubMed ID: 15031930
TITLE: Effect of transgenic Bt rice planting on soil enzyme activities.
AUTHOR: Sun Caixia; Chen Lijun; Wu Zhijie; Zhang Yulan; Zhang Lili
CORPORATE SOURCE: Institute of Applied Ecology, Chinese Academy of Sciences, Shenyang 110016, China.. suncaixia@hotmail.com
SOURCE: Ying yong sheng tai xue bao = journal of applied ecology / Zhongguo sheng tai xue xue hui, Zhongguo ke xue yuan Shenyang ying yong sheng tai yan jiu suo zhu ban, (2003 Dec) 14 (12) 2261-4.
Journal code: 9425159. ISSN: 1001-9332.
PUB. COUNTRY: China
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: Chinese
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200404
ENTRY DATE: Entered STN: 20040323
Last Updated on STN: 20040423
Entered Medline: 20040422

AB A pot experiment was conducted with silty loam Agrodolf as test soil and with transgenic Bt rice and non-Bt rice as test crops to study the effect of transgenic Bt rice planting on soil urease, phosphatase, arylsulfatase, invertase, and dehydrogenase activities. The results showed that Bt toxin could be introduced into soil through root exudates of transgenic Bt rice, and its survival amount in soil varied with time. Compared with non-Bt rice treatment, transgenic Bt rice treatment had a significant decrease (2.47%) of soil urease activity and a significant increase (8.91%) of soil **acid phosphatase** activity, but no significant change in soil arylsulfatase, invertase, and dehydrogenase activities at the 15th day of emergence. At the 30th day of emergence, the transgenic Bt rice treatment still had a significant decrease of soil urease activity (16.36%) and a significant increase of **acid phosphatase** activity (35.69%), and no change in invertase activity. It also had

significant increase in soil arylsulfatase (19.70%) and dehydrogenase activities (16.83%).

L38 ANSWER 6 OF 49 SCISEARCH COPYRIGHT 2004 THOMSON ISI on STN DUPLICATE 3
ACCESSION NUMBER: 2003:815767 SCISEARCH
THE GENUINE ARTICLE: 723VA
TITLE: Expression, purification, crystallization and preliminary
X-ray diffraction studies of recombinant
class B non-specific **acid phosphatase**
of Salmonella typhimurium
AUTHOR: Makde R D; Kumar V (Reprint); Gupta G D; Jasti J; Singh T
P; Mahajan S K
CORPORATE SOURCE: Bhabha Atom Res Ctr, Synchrotron Radiat Sect, Bombay
400085, Maharashtra, India (Reprint); All India Inst Med
Sci, Dept Biophys, New Delhi 110029, India; Bhabha Atom
Res Ctr, Div Mol Biol & Agr, Bombay 400085, Maharashtra,
India
COUNTRY OF AUTHOR: India
SOURCE: ACTA CRYSTALLOGRAPHICA SECTION D-BIOLOGICAL
CRYSTALLOGRAPHY, (OCT 2003) Vol. 59, Part 10, pp.
1849-1852.
Publisher: BLACKWELL MUNKSGAARD, 35 NORRE SOGADE, PO BOX
2148, DK-1016 COPENHAGEN, DENMARK.
ISSN: 0907-4449.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 25

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB The aphA gene of Salmonella enterica sv. Typhimurium strain MD6001 was
cloned in the multicopy plasmid pBluescript SK-. The recombinant AphA
protein was purified to homogeneity. The protein crystallized in the
orthorhombic space group P2(1)2(1)2(1), with unit-cell parameters a =
112.4, b = 130.2, c = 139.6 Angstrom. Consistent with the self-rotation
function, there are two tetramers in the asymmetric unit, indicating a
solvent content of similar to 54%. The **crystals** are composed of
biologically active AphA molecules.

L38 ANSWER 7 OF 49 MEDLINE on STN DUPLICATE 4
ACCESSION NUMBER: 2003084265 MEDLINE
DOCUMENT NUMBER: PubMed ID: 12595266
TITLE: Structure and function of an archaeal homolog of survival
protein E (SurEalpha): an **acid**
phosphatase with purine nucleotide specificity.
COMMENT: Erratum in: J Mol Biol. 2003 Apr 25;328(2):517
AUTHOR: Mura Cameron; Katz Jonathan E; Clarke Steven G; Eisenberg
David
CORPORATE SOURCE: Howard Hughes Medical Institute and UCLA-DOE Institute for
Genomics and Proteomics, Molecular Biology Institute, 201
Boyer Hall, Box 951570, Los Angeles, CA 90095-1570, USA.
CONTRACT NUMBER: AG18000 (NIA)
GM26020 (NIGMS)
SOURCE: Journal of molecular biology, (2003 Mar 7) 326 (5) 1559-75.
Journal code: 2985088R. ISSN: 0022-2836.
PUB. COUNTRY: England: United Kingdom
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200304
ENTRY DATE: Entered STN: 20030222
Last Updated on STN: 20030423
Entered Medline: 20030422

AB The survival protein E (SurE) family was discovered by its correlation to
stationary phase survival of Escherichia coli and various repair proteins
involved in sustaining this and other stress-response phenotypes. In
order to better understand this ancient and well-conserved protein family,
we have determined the 2.0A resolution **crystal** structure of
SurEalpha from the hyperthermophilic crenarchaeon Pyrobaculum aerophilum
(Pae). This first structure of an archaeal SurE reveals significant
similarities to and differences from the only other known SurE structure,
that from the eubacterium Thermatoga maritima (Tma). Both SurE monomers
adopt similar folds; however, unlike the Tma SurE dimer, crystalline Pae

SurEalpha is predominantly non-domain swapped. Comparative structural analyses of Tma and Pae SurE suggest conformationally variant regions, such as a hinge loop that may be involved in domain swapping. The putative SurE active site is highly conserved, and implies a model for SurE bound to a potential substrate, guanosine-5'-monophosphate (GMP). Pae SurEalpha has optimal **acid phosphatase** activity at temperatures above 90 degrees C, and is less specific than Tma SurE in terms of metal ion requirements. Substrate specificity also differs between Pae and Tma SurE, with a more specific recognition of purine nucleotides by the archaeal enzyme. Analyses of the sequences, phylogenetic distribution, and genomic organization of the SurE family reveal examples of genomes encoding multiple surE genes, and suggest that SurE homologs constitute a broad family of enzymes with **phosphatase-like** activities.

L38 ANSWER 8 OF 49 SCISEARCH COPYRIGHT 2004 THOMSON ISI on STN DUPLICATE 5
 ACCESSION NUMBER: 2003:438967 SCISEARCH
 THE GENUINE ARTICLE: 681PC
 TITLE: Expression, purification, crystallization and preliminary **X-ray** characterization of the class B **acid phosphatase** (AphA) from *Escherichia coli*
 AUTHOR: Forleo C; Benvenuti M; Calderone V; Schippa S; Docquier J D; Thaller M C; Rossolini G M; Mangani S (Reprint)
 CORPORATE SOURCE: Univ Siena, Dipartimento Chim, I-53100 Siena, Italy (Reprint); Univ Roma La Sapienza, Sez Microbiol, Dipartimento Sci Sanita Pubbl, Rome, Italy; Univ Siena, Dipartimento Biol Mol, I-53100 Siena, Italy; Univ Roma Tor Vergata, Dipartimento Biol, I-00173 Rome, Italy
 COUNTRY OF AUTHOR: Italy
 SOURCE: ACTA CRYSTALLOGRAPHICA SECTION D-BIOLOGICAL CRYSTALLOGRAPHY, (JUN 2003) Vol. 59, Part 6, pp. 1058-1060
 Publisher: BLACKWELL MUNKSGAARD, 35 NORRE SOGADE, PO BOX 2148, DK-1016 COPENHAGEN, DENMARK.
 ISSN: 0907-4449.
 DOCUMENT TYPE: Article; Journal
 LANGUAGE: English
 REFERENCE COUNT: 15

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB The class B non-specific **acid phosphatase** AphA from *Escherichia coli* has been expressed in *E. coli* and purified following a new protocol. ESI mass spectroscopy shows that the purified enzyme solution contains two polypeptides with molecular weights differing by 185 Da corresponding to two different cleavage sites of the signal peptide from the AphA *E. coli* precursor. Despite the solution heterogeneity, **X-ray** quality **crystals** have been obtained. However, the **crystals** have a tendency to give polymorphs and to lose long-range order with time while maintaining an intact **crystal** habit. **Crystals** have been grown in space groups I222 and C2 with three different unit cells and different asymmetric unit contents. Diffraction data to 1.6 Angstrom resolution have been collected with synchrotron radiation at ESRF and DESY.

L38 ANSWER 9 OF 49 SCISEARCH COPYRIGHT 2004 THOMSON ISI on STN DUPLICATE 6
 ACCESSION NUMBER: 2003:248115 SCISEARCH
 THE GENUINE ARTICLE: 656LT
 TITLE: Purification, crystallization and preliminary **X-ray** diffraction studies of recombinant class A non-specific **acid phosphatase** of *Salmonella typhimurium*
 AUTHOR: Makde R D; Kumar V (Reprint); Rao A S; Yadava V S; Mahajan S K
 CORPORATE SOURCE: Bhabha Atom Res Ctr, Synchrotron Radiat Sect, Bombay 400085, Maharashtra, India (Reprint); Bhabha Atom Res Ctr, Div Mol Biol & Agr, Bombay 400085, Maharashtra, India; Bhabha Atom Res Ctr, Div Solid State Phys, Bombay 400085, Maharashtra, India
 COUNTRY OF AUTHOR: India
 SOURCE: ACTA CRYSTALLOGRAPHICA SECTION D-BIOLOGICAL CRYSTALLOGRAPHY, (MAR 2003) Vol. 59, Part 3, pp. 515-518.

Publisher: BLACKWELL MUNKSGAARD, 35 NORRE SOGADE, PO BOX
2148, DK-1016 COPENHAGEN, DENMARK.
ISSN: 0907-4449.

DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 18

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB The *phoN* gene of *Salmonella enterica* sv. Typhimurium strain MD6001 was cloned in the multicopy plasmid pBluescript SK-. The nucleotide sequence of the cloned gene differs from the corresponding *S. typhimurium* LT2 sequence at 23 residues, leading to 15 amino-acid differences, but was very close to the *S. typhi* *phoN* sequence (only three nucleotide and two amino-acid differences). The recombinant PhoN protein was purified to homogeneity. Two forms of **crystals** were harvested from a single crystallization condition. Diffraction intensity data were collected using a laboratory **X-ray** source to resolution limits of 2.5 and 2.8 Angstrom for **crystals** belonging to space group C2 and C222(1), respectively. Based on noncrystallographic symmetry, four monomers of PhoN are expected to be present in the asymmetric unit of the C2 unit cell. Two monomers of a biologically active dimer in the asymmetric unit of the C222(1) unit cell are expected from the Matthews coefficient.

L38 ANSWER 10 OF 49 SCISEARCH COPYRIGHT 2004 THOMSON ISI on STN

ACCESSION NUMBER: 2003:120313 SCISEARCH

THE GENUINE ARTICLE: 637ZZ

TITLE: Structures of phosphate and trivanadate complexes of
Bacillus stearothermophilus **phosphatase** PhoE:
Structural and functional analysis in the

cofactor-dependent phosphoglycerate mutase superfamily
AUTHOR: Rigden D J; Littlejohn J E; Henderson K; Jedrzejewski M J
(Reprint)

CORPORATE SOURCE: Childrens Hosp Oakland Res Inst, 5700 Martin Luther King
Jr Way, Oakland, CA 94609 USA (Reprint); Childrens Hosp
Oakland Res Inst, Oakland, CA 94609 USA; Univ Calif
Berkeley, Lawrence Berkeley Lab, Berkeley Ctr Struct Biol,
Berkeley, CA 94720 USA; SAIN, EMBRAPA, Cenargen, Natl Ctr
Genet Resources & Biotechnol, BR-70770900 Brasilia, DF,
Brazil

COUNTRY OF AUTHOR: USA; Brazil

SOURCE: JOURNAL OF MOLECULAR BIOLOGY, (17 JAN 2003) Vol. 325, No.
3, pp. 411-420.

Publisher: ACADEMIC PRESS LTD ELSEVIER SCIENCE LTD, 24-28
OVAL RD, LONDON NW1 7DX, ENGLAND.

ISSN: 0022-2836.

DOCUMENT TYPE: Article; Journal

LANGUAGE: English

REFERENCE COUNT: 40

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB *Bacillus stearothermophilus* **phosphatase** PhoE is a member of the cofactor-dependent phosphoglycerate mutase superfamily possessing broad specificity **phosphatase** activity. Its previous structural determination in complex with glycerol revealed probable bases for its efficient hydrolysis of both large, hydrophobic, and smaller, hydrophilic substrates. Here we report two further structures of PhoE complexes, to higher resolution of diffraction, which yield a better and thorough understanding of its catalytic mechanism. The environment of the phosphate ion in the catalytic site of the first complex strongly suggests an acid-base catalytic function for Glu83. It also reveals how the C-terminal tail ordering is linked to enzyme activation on phosphate binding by a different mechanism to that seen in *Escherichia coli* phosphoglycerate mutase. The second complex structure with an unusual doubly covalently bound trivanadate shows how covalent modification of the phosphorylatable His10 is accompanied by small structural changes, presumably to catalytic advantage.

When compared with structures of related proteins in the cofactor-dependent phosphoglycerate mutase superfamily, an additional phosphate ligand, Gln22, is observed in PhoE. Functional constraints lead to the corresponding residue being conserved as Gly in fructose-2,6-bisphosphatases and Thr/Ser/Cys in phosphoglycerate mutases. A number of sequence annotation errors in databases are highlighted by

this analysis. B. stearothermophilus PhoE is evolutionarily related to a group of enzymes primarily present in Gram-positive bacilli. Even within this group substrate specificity is clearly variable highlighting the difficulties of computational functional annotation in the cofactor-dependent phosphoglycerate mutase superfamily. (C) 2003 Elsevier Science Ltd. All rights reserved.

L38 ANSWER 11 OF 49 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
ACCESSION NUMBER: 2003:406004 BIOSIS
DOCUMENT NUMBER: PREV200300406004
TITLE: **Crystal structure of AphA class B acid phosphatase/phosphotransferase from E. coli.**
AUTHOR(S): Calderone, Vito [Reprint Author]; Forleo, Costantino; Benvenuti, Manuela [Reprint Author]; Rossolini, Gian M.; Mangani, Stefano [Reprint Author]; Thaller, Maria C.
CORPORATE SOURCE: Dept of Chemistry, University of Siena, Siena, Italy
SOURCE: Journal of Inorganic Biochemistry, (15 July 2003) Vol. 96, No. 1, pp. 111. print.
Meeting Info.: 11th International Conference on Biological Inorganic Chemistry. Cairns, Australia. July 19-23, 2003. ISSN: 0162-0134 (ISSN print).
DOCUMENT TYPE: Conference; (Meeting)
Conference; (Meeting Poster)
Conference; Abstract; (Meeting Abstract)
LANGUAGE: English
ENTRY DATE: Entered STN: 3 Sep 2003
Last Updated on STN: 3 Sep 2003

L38 ANSWER 12 OF 49 SCISEARCH COPYRIGHT 2004 THOMSON ISI on STN
ACCESSION NUMBER: 2003:175274 SCISEARCH
THE GENUINE ARTICLE: 645YY
TITLE: Unexpected catalytic site variation in phosphoprotein **phosphatase** homologues of cofactor-dependent phosphoglycerate mutase
AUTHOR: Rigden D J (Reprint)
CORPORATE SOURCE: EMBRAPA, Cenargen, Embrapa Genet Resources & Biotechnol, Parque Estacao Biol, Final W3 Norte, BR-70770900 Brasilia, DF, Brazil (Reprint); EMBRAPA, Cenargen, Embrapa Genet Resources & Biotechnol, BR-70770900 Brasilia, DF, Brazil
COUNTRY OF AUTHOR: Brazil
SOURCE: FEBS LETTERS, (11 FEB 2003) Vol. 536, No. 1-3, pp. 77-84. Publisher: ELSEVIER SCIENCE BV, PO BOX 211, 1000 AE AMSTERDAM, NETHERLANDS. ISSN: 0014-5793.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 46

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB The cofactor-dependent phosphoglycerate mutase (dPGM) superfamily contains, besides mutases, a variety of **phosphatases**, both broadly and narrowly substrate-specific. Distant dPGM homologues, conspicuously abundant in microbial genomes, represent a challenge for functional annotation based on sequence comparison alone. Here we carry out sequence analysis and molecular modelling of two families of **bacterial** dPGM homologues, one the SixA phosphoprotein **phosphatases**, the other containing various proteins of no known molecular function. The models show how SixA proteins have adapted to phosphoprotein substrate and suggest that the second family may also encode phosphoprotein **phosphatases**. Unexpected variation in catalytic and substrate-binding residues is observed in the models. (C) 2003 Published by Elsevier Science B.V. on behalf of the Federation of European Biochemical Societies.

L38 ANSWER 13 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:937303 CAPLUS
DOCUMENT NUMBER: 138:20443
TITLE: Endocrine disruptor screening using DNA chips of endocrine disruptor-responsive genes
INVENTOR(S): Kondo, Akihiro; Takeda, Takeshi; Mizutani, Shigetoshi; Tsujimoto, Yoshimasa; Takashima, Ryokichi; Enoki, Yuki; Kato, Ikunoshin

PATENT ASSIGNEE(S): Takara Bio Inc., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 386 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002355079	A2	20021210	JP 2002-69354	20020313
PRIORITY APPLN. INFO.:			JP 2001-73183	A 20010314
			JP 2001-74993	A 20010315
			JP 2001-102519	A 20010330

AB A method and kit for detecting endocrine-disrupting chems. using DNA microarrays are claimed. The method comprises prepg. a nucleic acid sample contg. mRNAs or cDNAs originating in cells, tissues, or organisms which have been brought into contact with a sample contg. the endocrine disruptor. The nucleic acid sample is hybridized with DNA microarrays having genes affected by the endocrine disruptor or DNA fragments originating in these genes have been fixed. The results obtained are then compared with the results obtained with the control sample to select the gene affected by the endocrine disruptor. Genes whose expression is altered by tri-Bu tin, 4-octaphenol, 4-nonylphenol, di-N-Bu phthalate, dichlorohexyl phthalate, octachlorostyrene, benzophenone, diethylhexyl phthalate, diethylstilbestrol (DES), and 17-.beta. estradiol (E2), were found in mice by DNA chip anal.

L38 ANSWER 14 OF 49 SCISEARCH COPYRIGHT 2004 THOMSON ISI on STN
 ACCESSION NUMBER: 2002:395127 SCISEARCH
 THE GENUINE ARTICLE: 548VQ
 TITLE: Bromoperoxidase activity of vanadate-substituted
acid phosphatases from *Shigella flexneri*
 and *Salmonella enterica* ser. typhimurium
 AUTHOR: Tanaka N; Dumay V; Liao Q N; Lange A J; Wever R (Reprint)
 CORPORATE SOURCE: Univ Amsterdam, Inst Mol Chem, Nieuwe Achtergracht 129,
 NL-1018 WS Amsterdam, Netherlands (Reprint); Univ
 Amsterdam, Inst Mol Chem, NL-1018 WS Amsterdam,
 Netherlands; Univ Minnesota, Sch Med, Dept Biochem Mol
 Biol & Biophys, Minneapolis, MN 55455 USA; Univ Minnesota,
 Coll Biol Sci, Minneapolis, MN USA
 COUNTRY OF AUTHOR: Netherlands; USA
 SOURCE: EUROPEAN JOURNAL OF BIOCHEMISTRY, (APR 2002) Vol. 269, No.
 8, pp. 2162-2167.
 Publisher: BLACKWELL PUBLISHING LTD, P O BOX 88, OSNEY
 MEAD, OXFORD OX2 ONE, OXON, ENGLAND.
 ISSN: 0014-2956.
 DOCUMENT TYPE: Article; Journal
 LANGUAGE: English
 REFERENCE COUNT: 28

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS
 AB Vanadium haloperoxidases and the **bacterial** class A nonspecific **acid phosphatases** have a conserved active site. It is shown that vanadate-substituted recombinant **acid phosphatase** from *Shigella flexneri* (PhoN-Sf) and *Salmonella enterica* ser. typhimurium (PhoN-Se) in the presence of H₂O₂ are able to oxidize bromide to hypobromous acid. Vanadate is essential for this activity. The kinetic parameters for the artificial bromoperoxidases have been determined. The K_m value for H₂O₂ is about the same as that for the vanadium bromoperoxidases from the seaweed *Ascophyllum nodosum*. However, the K_m value for Br⁻ is about 10-20 times higher, and the turnover values of about 3.4 min⁻¹ and 33 min⁻¹ for PhoN-Sf and PhoN-Se, respectively, are much slower, than those of the native bromoperoxidase. Thus, despite the striking similarity in the active-site structures of the vanadium haloperoxidases and the acid phosphatase, the turnover frequency is low, and clearly the active site of **acid phosphatases** is not optimized for haloperoxidase activity. Like the native vanadium bromoperoxidase, the vanadate-substituted PhoN-Sf and PhoN-Se catalyse the enantioselective sulfoxidation of thioanisole.

L38 ANSWER 15 OF 49 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

DUPLICATE 7
 ACCESSION NUMBER: 2002:371624 BIOSIS
 DOCUMENT NUMBER: PREV200200371624
 TITLE: Mechanistic implications for Escherichia coli cofactor-dependent phosphoglycerate mutase based on the high-resolution **crystal** structure of a vanadate complex.
 AUTHOR(S): Bond, Charles S.; White, Malcolm F.; Hunter, William N. [Reprint author]
 CORPORATE SOURCE: Division of Biological Chemistry and Molecular Microbiology, Wellcome Trust Biocentre, University of Dundee, Dundee, DD1 5EH, UK
 W.N.Hunter@dundee.ac.uk
 SOURCE: Journal of Molecular Biology, (8 March, 2002) Vol. 316, No. 5, pp. 1071-1081. print.
 CODEN: JMOBAK. ISSN: 0022-2836.
 DOCUMENT TYPE: Article
 LANGUAGE: English
 ENTRY DATE: Entered STN: 3 Jul 2002
 Last Updated on STN: 3 Jul 2002
 AB The structure of Escherichia coli cofactor-dependent phosphoglycerate mutase (dPGM), complexed with the potent inhibitor vanadate, has been determined to a resolution of 1.30 Å (R-factor 0.159; R-free 0.213). The inhibitor is present in the active site, principally as divanadate, but with evidence of additional vanadate moieties at either end, and representing a different binding mode to that observed in the structural homologue prostatic **acid phosphatase**. The analysis reveals the enzyme-ligand interactions involved in inhibition of the mutase activity by vanadate and identifies a water molecule, observed in the native E. coli dPGM structure which, once activated by vanadate, may dephosphorylate the active protein. Rather than reflecting the active conformation previously observed for E. coli dPGM, the inhibited protein's conformation resembles that of the inactive dephosphorylated Saccharomyces cerevisiae dPGM. The provision of a high-resolution structure of both active and inactive forms of dPGM from a single organism, in conjunction with computational modelling of substrate molecules in the active site provides insight into the binding of substrates and the specific interactions necessary for three different activities, mutase, synthase and **phosphatase**, within a single active site. The sequence similarity of E. coli and human dPGMs allows us to correlate structure with clinical pathology.

L38 ANSWER 16 OF 49 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
 ACCESSION NUMBER: 2002:546807 BIOSIS
 DOCUMENT NUMBER: PREV200200546807
 TITLE: Enhancement of nucleoside phosphorylation activity in an **acid phosphatase**.
 AUTHOR(S): Ishikawa, Kohki; Mihara, Yasuhiro; Shimba, Nobuhisa; Ohtsu, Naoko; Kawasaki, Hisashi; Suzuki, Ei-ichiro [Reprint author]; Asano, Yasuhisa
 CORPORATE SOURCE: Central Research Laboratories, Ajinomoto Co., Inc., 1-1 Suzuki-cho Kawasaki-ku, Kawasaki, 210-8681, Japan
 SOURCE: Protein Engineering, (July, 2002) Vol. 15, No. 7, pp. 539-543. print.
 CODEN: PRENE9. ISSN: 0269-2139.
 DOCUMENT TYPE: Article
 LANGUAGE: English
 ENTRY DATE: Entered STN: 23 Oct 2002
 Last Updated on STN: 23 Oct 2002
 AB Escherichia blattae non-specific **acid phosphatase** (EB-NSAP) possesses a pyrophosphate-nucleoside phosphotransferase activity, which is C-5'-position selective. Current mutational and structural data were used to generate a mutant EB-NSAP for a potential industrial application as an effective and economical protein catalyst in synthesizing nucleotides from nucleosides. First, Gly74 and Ile153 were replaced by Asp and Thr, respectively, since the corresponding replacements in the homologous enzyme from Morganella morganii reduced the Km value for inosine and thus increased the productivity of 5'-IMP. We determined the **crystal** structure of G74D/I153T, which has a reduced Km value for inosine, as expected. The tertiary structure of G74D/I153T was virtually identical to that of the wild-type. In addition,

neither of the introduced side chains of Asp74 and Thr153 is directly involved in the interaction with inosine in a hypothetical binding mode of inosine to EB-NSAP, although both residues are situated near a potential inosine-binding site. These findings suggested that a slight structural change caused by an amino acid replacement around the potential inosine-binding site could significantly reduce the Km value. Prompted by this hypothesis, we designed several mutations and introduced them to G74D/I153T, to decrease the Km value further. This strategy produced a S72F/G74D/I153T mutant with a 5.4-fold lower Km value and a 2.7-fold higher Vmax value as compared to the wild-type EB-NSAP.

L38 ANSWER 17 OF 49 MEDLINE on STN
 ACCESSION NUMBER: 2002323777 MEDLINE
 DOCUMENT NUMBER: PubMed ID: 12029286
 TITLE: A mouse model of inflammatory root resorption induced by pulpal infection.
 AUTHOR: Balto Khaled; White Robert; Mueller Ralph; Stashenko Philip
 CORPORATE SOURCE: Department of Cytokine Biology, Forsyth Institute, Boston, Mass 02115, USA.
 CONTRACT NUMBER: AG-13333 (NIA)
 DE-09018 (NIDCR)
 DE-11664 (NIDCR)
 DE-13747 (NIDCR)
 SOURCE: Oral surgery, oral medicine, oral pathology, oral radiology, and endodontics, (2002 Apr) 93 (4) 461-8.
 Journal code: 9508562. ISSN: 1079-2104.
 PUB. COUNTRY: United States
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 LANGUAGE: English
 FILE SEGMENT: Dental Journals; Priority Journals
 ENTRY MONTH: 200210
 ENTRY DATE: Entered STN: 20020618
 Last Updated on STN: 20021004
 Entered Medline: 20021003

AB OBJECTIVE: The present study was undertaken to determine the frequency and extent of apical root resorption associated with induced periradicular lesions in mice. STUDY DESIGN: Bone and root resorption was quantified by using two- and three-dimensional micro-computed tomography (mu-CT) in the lower first molars of mice subjected to pulp exposure and infection. RESULTS: mu-CT measurements showed significant apical resorption in exposed and infected teeth, resulting in an average distal root shortening of 12.7% (P < .001 vs unexposed). These findings were confirmed with three-dimensional reconstituted images that showed thinning and shortening of the distal root. Tartrate-resistant **acid phosphatase** clastic cells were associated with resorption lacunae on the cementum of root apices, as well as on bone at the periphery of the periradicular lesions. Brown and Brenn staining showed the presence of **bacteria** in dentinal tubules adjacent to resorbed cementum. CONCLUSIONS: Apical root resorption is a prominent and consistent finding associated with periradicular infection in the mouse. This species represents a convenient model for studying the pathogenesis of inflammatory root resorption in vivo.

L38 ANSWER 18 OF 49 SCISEARCH COPYRIGHT 2004 THOMSON ISI on STN
 ACCESSION NUMBER: 2002:135593 SCISEARCH
 THE GENUINE ARTICLE: 518CE
 TITLE: 3 ',5 '-cyclic nucleotide phosphodiesterases class III: Members, structure, and catalytic mechanism
 AUTHOR: Richter W (Reprint)
 CORPORATE SOURCE: Stanford Univ, Sch Med, Div Reprod Biol, Dept Gynecol & Obstet, 300 Pasteur Dr, Stanford, CA 94305 USA (Reprint);
 Stanford Univ, Sch Med, Div Reprod Biol, Dept Gynecol & Obstet, Stanford, CA 94305 USA
 COUNTRY OF AUTHOR: USA
 SOURCE: PROTEINS-STRUCTURE FUNCTION AND GENETICS, (15 FEB 2002)
 Vol. 46, No. 3, pp. 278-286.
 Publisher: WILEY-LISS, DIV JOHN WILEY & SONS INC, 605 THIRD AVE, NEW YORK, NY 10158-0012 USA.
 ISSN: 0887-3585.
 DOCUMENT TYPE: Article; Journal
 LANGUAGE: English

REFERENCE COUNT:

44

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB 3',5'-Cyclic nucleotide phosphodiesterases (PDEs) comprise a superfamily of enzymes that were previously divided by their primary structure into two major classes: PDE class I and II. The 3',5'-cyclic AMP phosphodiesterase from *Escherichia coli* encoded by the *cpdA* gene does not show any homology to either PDE class I or class II enzymes and, therefore, represents a new, third class of PDEs. Previously, information about essential structural elements, substrate and cofactor binding sites, and the mechanism of catalysis was unknown for this enzyme. The present study shows by computational analysis that the enzyme encoded by the *E. coli cpdA* gene belongs to a family of phosphodiesterases that closely resembles the catalytic machinery known from purple **acid phosphatases** and several other dimetallophosphoesterases. They share both the conserved sequence motif, D-(X)(n)-GD-(X)(n)-GNH[E/D]-(X)(n)-H-(X)(n)-GHXH, which contains the invariant residues forming the active site of purple **acid phosphatases**, a binuclear Fe3+-Mg2+-containing center, as well as a betaalphanbetapheta motif as a typical secondary structure signature. Furthermore, the known biochemical properties of the **bacterial** phosphodiesterase encoded by the *cpdA* gene, such as the requirement of iron ions and a reductant for maintaining its catalytic activity, support this hypothesis developed by computational analysis. In addition, the availability of atomic coordinates for several purple **acid phosphatases** and related proteins allowed the generation of a three-dimensional model for class III cyclic nucleotide phosphodiesterases. (C) 2002 Wiley-Liss, Inc.

L38 ANSWER 19 OF 49 SCISEARCH COPYRIGHT 2004 THOMSON ISI on STN DUPLICATE 8

ACCESSION NUMBER: 2001:862257 SCISEARCH

THE GENUINE ARTICLE: 486CP

TITLE: MDP-1 is a new and distinct member of the haloacid dehalogenase family of aspartate-dependent phosphohydrolases

AUTHOR: Selengut J D (Reprint)

CORPORATE SOURCE: NHLBI, Biochem Lab, NIH, 50 South Dr, Bldg 50-2347, Bethesda, MD 20892 USA (Reprint); NHLBI, Biochem Lab, NIH, Bethesda, MD 20892 USA

COUNTRY OF AUTHOR: USA

SOURCE: BIOCHEMISTRY, (23 OCT 2001) Vol. 40, No. 42, pp. 12704-12711.

Publisher: AMER CHEMICAL SOC, 1155 16TH ST, NW,

WASHINGTON, DC 20036 USA.

ISSN: 0006-2960.

DOCUMENT TYPE: Article; Journal

LANGUAGE: English

REFERENCE COUNT: 26

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB MDP-1 is a eukaryotic magnesium-dependent **acid phosphatase** with little sequence homology to previously characterized **phosphatases**. The presence of a conserved motif (Asp-X-Asp-X-Thr) in the N terminus of MDP-1 suggested a relationship to the haloacid dehalogenase (HAD) superfamily, which contains a number of magnesium-dependent **acid phosphatases**. These **phosphatases** utilize an aspartate nucleophile and contain a number of conserved active-site residues and hydrophobic patches, which can be plausibly aligned with conserved residues in MDP-1. Seven site-specific point mutants of MDP-I were produced by modifying the catalytic aspartate, serine, and lysine residues to asparagine or glutamate, alanine, and arginine, respectively. The activity of these mutants confirms the assignment of MDP-I as a member of the HAD superfamily. Detailed comparison of the sequence of the 15 MDP-I sequences from various organisms with other HAD superfamily sequences suggests that MDP-I is not closely related to any particular member of the superfamily. The **crystal** structures of several HAD family enzymes identify a domain proximal to the active site responsible for important interactions with low molecular weight substrates. The absence of this domain or any other that might perform the same function in MDP-1 suggests an "open" active site capable of interactions with large substrates such as proteins. This suggestion was experimentally confirmed by demonstration that MDP-I is competent to catalyze the dephosphorylation of tyrosine-phosphorylated

proteins.

L38 ANSWER 20 OF 49 SCISEARCH COPYRIGHT 2004 THOMSON ISI on STN
ACCESSION NUMBER: 2001:730461 SCISEARCH
THE GENUINE ARTICLE: 469NJ
TITLE: A cofactor-dependent phosphoglycerate mutase homolog from
Bacillus stearothermophilus is actually a broad
specificity **phosphatase**
AUTHOR: Rigden D J; Bagyan I; Lamani E; Setlow P; Jedrzejewski M J
(Reprint)
CORPORATE SOURCE: Childrens Hosp Oakland Res Inst, 5700 Martin Luther King
Jr Way, Oakland, CA 94609 USA (Reprint); EMBRAPA,
Cenargen, Natl Ctr Genet Resources & Biotechnol,
BR-70770900 Brasilia, DF, Brazil; Univ Connecticut, Ctr
Hlth, Dept Biochem, Farmington, CT 06032 USA; Univ
Alabama, Dept Microbiol, Birmingham, AL 35294 USA
COUNTRY OF AUTHOR: USA; Brazil
SOURCE: PROTEIN SCIENCE, (SEP 2001) Vol. 10, No. 9, pp. 1835-1846.
Publisher: COLD SPRING HARBOR LAB PRESS, 1 BUNGTOWN RD,
PLAINVIEW, NY 11724 USA.
ISSN: 0961-8368.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 60

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB The distribution of phosphoglycerate mutase (PGM) activity in
bacteria is complex, with some organisms possessing, both a
cofactor-dependent and a cofactor-independent PGM and others having only
one of these enzymes. Although Bacillus species contain only a
cofactor-independent PGM, genes homologous to those encoding
cofactor-dependent PGMs have been detected in this group of
bacteria, but in at least one case the encoded protein lacks
significant PGM activity. Here we apply sequence analysis, molecular
modeling, and enzymatic assays to the cofactor-dependent PGM homologs from
B. stearothermophilus and B. subtilis, and show that these enzymes are
phosphatases with broad substrate specificity. Homologs from other
grampositive **bacteria** are also likely to possess
phosphatase activity. These studies clearly show that the
exploration of genomic sequences through three-dimensional modeling is
capable of producing useful predictions regarding function. However,
significant methodological improvements will be needed before such
analysis can be carried out automatically.

L38 ANSWER 21 OF 49 SCISEARCH COPYRIGHT 2004 THOMSON ISI on STN
ACCESSION NUMBER: 2001:488103 SCISEARCH
THE GENUINE ARTICLE: 440UZ
TITLE: Substrate analysis and molecular cloning of the
extracellular alkaline **phosphatase** of
Streptomyces griseus
AUTHOR: Moura R S; Martin J F; Martin A; Liras P (Reprint)
CORPORATE SOURCE: Inst Biotecnol Leon INBIOTEC, Parque Cient Leon, Avda del
Real 1, Leon 24006, Spain (Reprint); Inst Biotecnol Leon
INBIOTEC, Leon 24006, Spain; Univ Leon, Fac Ciencias Biol
& Ambientales, Area Microbiol, E-24071 Leon, Spain
COUNTRY OF AUTHOR: Spain
SOURCE: MICROBIOLOGY-SGM, (JUN 2001) Vol. 147, Part 6, pp.
1525-1533.
Publisher: SOC GENERAL MICROBIOLOGY, MARLBOROUGH HOUSE,
BASINGSTOKE RD, SPENCERS WOODS, READING RG7 1AE, BERKS,
ENGLAND.
ISSN: 1350-0872.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 42

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB Streptomyces species secrete large amounts of alkaline
phosphatase (AP) enzymes that have not been characterized so far.
An AP has been purified to homogeneity from cultures of Streptomyces
griseus IMRU 3570. The enzyme has a monomer size of 62 kDa and is
processed in the culture to a 33 kDa protein as shown by immunoblotting.
The enzyme was purified by ammonium sulfate precipitation. CM-Sephadex

cationic exchange, chromatofocusing and HPLC Sphaerogel 3000SW filtration, The pure enzyme uses a variety of organic phosphorylated compounds as substrates, The N-terminal end of the mature protein was found to be RLREDPFETLGVASGDPHP. The gene phoA has been cloned using as probe an oligomer based on the N-terminal sequence of the *S. griseus* AP, phoA encodes a protein of 62 678 Da with low homology to the AP of *Escherichia coli*, The phoA gene was found to be homologous to three alkaline-**phosphatase**-encoding genes previously identified in the *Streptomyces coelicolor* genome. On the basis of the optimal pH, substrate specificity and differences in amino acid sequence of motifs defining the active centre of APs, the *S. griseus* AP uses a wide range of organic phosphate substrates and is different from the **phosphatases** of Gram-negative **bacteria**.

L38 ANSWER 22 OF 49 MEDLINE on STN DUPLICATE 9
 ACCESSION NUMBER: 2001664024 MEDLINE
 DOCUMENT NUMBER: PubMed ID: 11709173
 TITLE: Structure of *Thermotoga maritima* stationary phase survival protein SurE: a novel **acid phosphatase**.
 AUTHOR: Zhang R G; Skarina T; Katz J E; Beasley S; Khachatryan A; Vyas S; Arrowsmith C H; Clarke S; Edwards A; Joachimiak A; Savchenko A
 CORPORATE SOURCE: Biosciences Division and Structural Biology Center, Argonne National Laboratory, 9700 South Cass Avenue, Building 202, Argonne, IL 60439, USA.
 CONTRACT NUMBER: GM-07135 (NIGMS)
 GM62414-01 (NIGMS)
 SOURCE: Structure (Cambridge, Mass. : 2001), (2001 Nov) 9 (11) 1095-106.
 Journal code: 101087697. ISSN: 0969-2126.
 PUB. COUNTRY: United States
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals
 OTHER SOURCE: PDB-1ILV
 ENTRY MONTH: 200202
 ENTRY DATE: Entered STN: 20011119
 Last Updated on STN: 20020212
 Entered Medline: 20020211

AB BACKGROUND: The *rpoS*, *nlpD*, *pcm*, and *surE* genes are among many whose expression is induced during the stationary phase of **bacterial** growth. *rpoS* codes for the stationary-phase RNA polymerase sigma subunit, and *nlpD* codes for a lipoprotein. The *pcm* gene product repairs damaged proteins by converting the atypical isoaspartyl residues back to L-aspartyls. The physiological and biochemical functions of *surE* are unknown, but its importance in stress is supported by the duplication of the *surE* gene in *E. coli* subjected to high-temperature growth. The *pcm* and *surE* genes are highly conserved in **bacteria**, archaea, and plants. RESULTS: The structure of SurE from *Thermotoga maritima* was determined at 2.0 Å. The SurE monomer is composed of two domains; a conserved N-terminal domain, a Rossman fold, and a C-terminal oligomerization domain, a new fold. Monomers form a dimer that assembles into a tetramer. Biochemical analysis suggests that SurE is an **acid phosphatase**, with an optimum pH of 5.5-6.2. The active site was identified in the N-terminal domain through analysis of conserved residues. Structure-based site-directed point mutations abolished **phosphatase** activity. *T. maritima* SurE intra- and intersubunit salt bridges were identified that may explain the SurE thermostability. CONCLUSIONS: The structure of SurE provided information about the protein's fold, oligomeric state, and active site. The protein possessed magnesium-dependent **acid phosphatase** activity, but the physiologically relevant substrate(s) remains to be identified. The importance of three of the assigned active site residues in catalysis was confirmed by site-directed mutagenesis.

L38 ANSWER 23 OF 49 MEDLINE on STN
 ACCESSION NUMBER: 2001481144 MEDLINE
 DOCUMENT NUMBER: PubMed ID: 11524683
 TITLE: **Crystal** structure and functional analysis of the SurE protein identify a novel **phosphatase** family.
 AUTHOR: Lee J Y; Kwak J E; Moon J; Eom S H; Liang E C; Pedelacq J

CORPORATE SOURCE: D; Berendzen J; Suh S W
School of Chemistry and Molecular Engineering, College of
Natural Sciences, Seoul National University, Seoul 151-742,
Korea.

SOURCE: Nature structural biology, (2001 Sep) 8 (9) 789-94.
Journal code: 9421566. ISSN: 1072-8368.

PUB. COUNTRY: United States

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

FILE SEGMENT: Priority Journals

OTHER SOURCE: PDB-1J9J; PDB-1J9K; PDB-1J9L

ENTRY MONTH: 200109

ENTRY DATE: Entered STN: 20010830
Last Updated on STN: 20011001
Entered Medline: 20010927

AB Homologs of the Escherichia coli surE gene are present in many eubacteria and archaea. Despite the evolutionary conservation, little information is available on the structure and function of their gene products. We have determined the **crystal** structure of the SurE protein from Thermotoga maritima. The structure reveals the dimeric arrangement of the subunits and an active site around a bound metal ion. We also demonstrate that the SurE protein exhibits a divalent metal ion-dependent **phosphatase** activity that is inhibited by vanadate or tungstate. In the vanadate- and tungstate-complexed structures, the inhibitors bind adjacent to the divalent metal ion. Our structural and functional analyses identify the SurE proteins as a novel family of metal ion-dependent **phosphatases**.

L38 ANSWER 24 OF 49 MEDLINE on STN

ACCESSION NUMBER: 2001270366 MEDLINE

DOCUMENT NUMBER: PubMed ID: 11264598

TITLE: Crystallization and preliminary **X-ray**
crystallographic analysis of the surE protein from
Thermotoga maritima.

AUTHOR: Kwak J E; Ha K S; Lee J Y; Im Y J; Park S H; Eom S H; Suh S
W

CORPORATE SOURCE: School of Chemistry and Molecular Engineering, Seoul
National University, Seoul 151-742, South Korea.

SOURCE: Acta crystallographica. Section D, Biological
crystallography, (2001 Apr) 57 (Pt 4) 612-3.
Journal code: 9305878. ISSN: 0907-4449.

PUB. COUNTRY: Denmark

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

FILE SEGMENT: Priority Journals

ENTRY MONTH: 200106

ENTRY DATE: Entered STN: 20010625
Last Updated on STN: 20010625
Entered Medline: 20010621

AB The surE protein from Thermotoga maritima is a 247-residue protein of unknown function. Its homologues are well conserved among both the eubacteria and the archaea. It has been overexpressed in soluble form in Escherichia coli. The protein has been crystallized at 296 K using 2-propanol as a precipitant. **X-ray** diffraction data have been collected to 1.9 Å resolution using synchrotron radiation. The **crystals** belong to the trigonal space group P3(1)21 (or P3(2)21), with unit-cell parameters a = b = 115.96, c = 78.60 Å, alpha = beta = 90, gamma = 120 degrees. The asymmetric unit contains two monomers of the surE protein, with a corresponding V(M) of 2.72 Å(3) Da(-1) and a solvent content of 54.7%.

L38 ANSWER 25 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 10

ACCESSION NUMBER: 2001:839804 CAPLUS

DOCUMENT NUMBER: 136:67142

TITLE: Lysosomes and sulfide-oxidizing bodies in the
bacteriocytes of Lucina pectinata, a cytochemical and
microanalysis approach

AUTHOR(S): Liberge, M.; Gros, O.; Frenkiel, L.

CORPORATE SOURCE: Universite des Antilles et de la Guyane, Departement
de Biologie, Pointe-a-Pitre, 97159, Fr.

SOURCE: Marine Biology (Berlin, Germany) (2001), 139(3),

401-409
 CODEN: MBIOAJ; ISSN: 0025-3162
 PUBLISHER: Springer-Verlag
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB L. pectinata is a large tropical clam living deeply burrowed in the black, reducing mud of mangrove swamps. It is known to possess Hb in the cytoplasmic areas of its bacteriocytes, which harbor sulfide-oxidizing **bacteria**. The bacteriocytes also possess lysosome-like microbodies contg. either membrane whorls or electron-dense granules in which free heme compds. have been identified. The cytochem. detection of **acid phosphatase** and arylsulfatase through EDX (energy-dispersive **x-ray**) microanal. strongly suggests that the bacteriocytes of L. pectinata contain, in fact, 2 different types of microbodies. Some of these (devoid of dense granules) possess a variable amt. of lysosomal enzymes and occasionally a limited quantity of iron, which may result from a recycling process of Hb. Their main function seems to be the digestion of a limited proportion of symbiotic **bacteria**. They represent genuine secondary lysosomes with a functionally acidic pH. The 2nd type of microbodies is characterized by dense granules contg. sulfur and iron hemes but no lysosomal enzymes. Their sulfide-oxidizing activity was substantiated by benzyl viologen assay, with Na₂S as a substrate. These microbodies appear to be similar to the sulfide-oxidizing bodies (SOBs) described in the bacteriocytes of other bivalve species with symbiotic thioautotrophic **bacteria**; however, their sulfide-oxidizing activity appears to be non-enzymic. They are discrete organelles, characterized by a functionally basic pH and pseudoperoxidasic activity, and have been termed SOBs. Therefore, the bacteriocytes of L. pectinata possess at the same time functional lysosomes and functional SOBs.

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 26 OF 49 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
 ACCESSION NUMBER: 2001:324292 BIOSIS
 DOCUMENT NUMBER: PREV200100324292
 TITLE: Mechanism of hydrolysis of phosphate esters by the dimetal center of 5'-nucleotidase based on **crystal** structures.

AUTHOR(S): Knoefel, Thomas [Reprint author]; Straeter, Norbert
 CORPORATE SOURCE: Abteilung Kristallographie, Institut fuer Chemie, Freie Universitaet Berlin, Takustrasse 6, 14195, Berlin, Germany
 strater@chemie.fu-berlin.de

SOURCE: Journal of Molecular Biology, (25 May, 2001) Vol. 309, No. 1, pp. 239-254. print.
 CODEN: JMOBAK. ISSN: 0022-2836.

DOCUMENT TYPE: Article
 LANGUAGE: English
 ENTRY DATE: Entered STN: 11 Jul 2001
 Last Updated on STN: 22 Feb 2002

AB 5'-Nucleotidase belongs to a large superfamily of distantly related dinuclear metallophosphatases including the Ser/Thr protein **phosphatases** and purple **acid phosphatases**. The protein undergoes a 96degree domain rotation between an open (inactive) and a closed (active) enzyme form. Complex structures of the closed form with the products adenosine and phosphate, and with the substrate analogue inhibitor alpha,beta-methylene ADP, have been determined at 2.1 ANG and 1.85 ANG resolution, respectively. In addition, a complex of the open form of 5'-nucleotidase with ATP was analyzed at a resolution of 1.7 ANG. These structures show that the adenosine group binds to a specific binding pocket of the C-terminal domain. The adenine ring is stacked between Phe429 and Phe498. The N-terminal domain provides the ligands to the dimetal cluster and the conserved His117, which together form the catalytic core structure. However, the three C-terminal arginine residues 375, 379 and 410, which are involved in substrate binding, may also play a role in transition-state stabilization. The beta-phosphate group of the inhibitor is terminally coordinated to the site 2 metal ion. The site 1 metal ion coordinates a water molecule which is in an ideal position for a nucleophilic attack on the phosphorus atom, assuming an in-line mechanism of phosphoryl transfer. Another water molecule bridges the two metal ions.

L38 ANSWER 27 OF 49 MEDLINE on STN DUPLICATE 11

ACCESSION NUMBER: 2000296667 MEDLINE
DOCUMENT NUMBER: PubMed ID: 10835340
TITLE: **X-ray** structures of a novel
acid phosphatase from *Escherichia blattae*
and its complex with the transition-state analog molybdate.
AUTHOR: Ishikawa K; Mihara Y; Gondoh K; Suzuki E; Asano Y
CORPORATE SOURCE: Central Research Laboratories, Ajinomoto Co., Inc., 1-1
Suzuki-cho, Kawasaki-ku, Kawasaki 210-8681, Japan.
SOURCE: EMBO journal, (2000 Jun 1) 19 (11) 2412-23.
Journal code: 8208664. ISSN: 0261-4189.
PUB. COUNTRY: ENGLAND: United Kingdom
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 200007
ENTRY DATE: Entered STN: 20000728
Last Updated on STN: 20000728
Entered Medline: 20000720

AB The structure of *Escherichia blattae* non-specific **acid phosphatase** (EB-NSAP) has been determined at 1.9 Å resolution with a bound sulfate marking the phosphate-binding site. The enzyme is a 150 kDa homohexamer. EB-NSAP shares a conserved sequence motif not only with several lipid **phosphatases** and the mammalian glucose-6-**phosphatases**, but also with the vanadium-containing chloroperoxidase (CPO) of *Curvularia inaequalis*. Comparison of the **crystal** structures of EB-NSAP and CPO reveals striking similarity in the active site structures. In addition, the topology of the EB-NSAP core shows considerable similarity to the fold of the active site containing part of the monomeric 67 kDa CPO, despite the lack of further sequence identity. These two enzymes are apparently related by divergent evolution. We have also determined the **crystal** structure of EB-NSAP complexed with the transition-state analog molybdate. Structural comparison of the native enzyme and the enzyme-molybdate complex reveals that the side-chain of His150, a putative catalytic residue, moves toward the molybdate so that it forms a hydrogen bond with the metal oxyanion when the molybdenum forms a covalent bond with NE2 of His189.

L38 ANSWER 28 OF 49 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: 2000:408500 BIOSIS
DOCUMENT NUMBER: PREV200000408500
TITLE: Enzymically mediated bioprecipitation of uranium by a
Citrobacter sp.: A concerted role for exocellular
lipopolysaccharide and associated **phosphatase** in
biomineral formation.
AUTHOR(S): Macaskie, Lynne E. [Reprint author]; Bonthron, Karen M.;
Yong, Ping; Goddard, David T.
CORPORATE SOURCE: School of Biosciences, University of Birmingham, Edgbaston,
Birmingham, B15 2TT, UK
SOURCE: Microbiology (Reading), (August, 2000) Vol. 146, No. 8, pp.
1855-1867. print.
ISSN: 1350-0872.
DOCUMENT TYPE: Article
LANGUAGE: English
ENTRY DATE: Entered STN: 27 Sep 2000
Last Updated on STN: 8 Jan 2002

AB A *Citrobacter* sp. accumulated uranyl ion (UO₂²⁺) via precipitation with phosphate ligand liberated by **phosphatase** activity. The onset and rate of uranyl phosphate deposition were promoted by NH₄⁺ forming NH₄UO₂PO₄, which has a lower solubility product than NaUO₂PO₄. This acceleration decoupled the rate-limiting chemical crystallization process from the biochemical phosphate ligand generation. This provided a novel approach to monitor the cell-surface-associated changes using atomic-force microscopy in conjunction with transmission electron microscopy and electron-probe **X-ray** microanalysis, to visualize deposition of uranyl phosphate at the cell surface. Analysis of extracted surface materials by ³¹P NMR spectroscopy showed phosphorus resonances at chemical shifts of 0.3 and 2.0 p.p.m., consistent with monophosphate groups of the lipid A backbone of the lipopolysaccharide (LPS). Addition of UO₂²⁺ to the extract gave a yellow precipitate which contained uranyl

phosphate, while addition of Cd²⁺ gave a chemical shift of both resonances to a single new resonance at 3 p.p.m. **Acid-phosphatase** -mediated **crystal** growth exocellularly was suggested by the presence of **acid phosphatase**, localized by immunogold labelling, on the outer membrane and on material exuded from the cells. Metal deposition is proposed to occur via an initial nucleation with phosphate groups localized within the LPS, shown by other workers to be produced exocellularly in association with **phosphatase**. The **crystals** are further consolidated with additional, enzymically generated phosphate in close juxtaposition, giving high loads of LPS-bound uranyl phosphate without loss of activity and distinguishing this from simple biosorption, or periplasmic or cellular metal accumulation mechanisms. Accumulation of 'tethered' metal phosphate within the LPS is suggested to prevent fouling of the cell surface by the accumulated precipitate and localization of **phosphatase** exocellularly is consistent with its possible functions in homeostasis and metal resistance.

L38 ANSWER 29 OF 49 SCISEARCH COPYRIGHT 2004 THOMSON ISI on STN
 ACCESSION NUMBER: 2000:782222 SCISEARCH
 THE GENUINE ARTICLE: 362KR
 TITLE: Purple **acid phosphatases** from

bacteria: similarities to mammalian and plant enzymes
 AUTHOR: Schenk G (Reprint); Korsinczky M L J; Hume D A; Hamilton S; DeJersey J
 CORPORATE SOURCE: UNIV QUEENSLAND, DEPT BIOCHEM, BRISBANE, QLD 4072, AUSTRALIA (Reprint); UNIV QUEENSLAND, INST MOL BIOSCI, BRISBANE, QLD 4072, AUSTRALIA
 COUNTRY OF AUTHOR: AUSTRALIA
 SOURCE: GENE, (19 SEP 2000) Vol. 255, No. 2, pp. 419-424. Publisher: ELSEVIER SCIENCE BV, PO BOX 211, 1000 AE AMSTERDAM, NETHERLANDS. ISSN: 0378-1119.
 DOCUMENT TYPE: Article; Journal
 FILE SEGMENT: LIFE
 LANGUAGE: English
 REFERENCE COUNT: 30

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB Mammalian and plant purple **acid phosphatases** have similar active site structures despite low sequence identity (<20%). Although no **bacterial** enzyme has been purified, a sequence database search revealed that genes that could encode potential purple **acid phosphatases** may be restricted to a small number of organisms (i.e., myco- and cyanobacteria). Analysis of their deduced amino acid sequences and predicted secondary structures indicates that the cyanobacterial enzyme is similar to both the mammalian and the recently discovered low-molecular-weight plant purple **acid phosphatases**, while the mycobacterial enzyme is homologous to the fungal and high-molecular-weight plant purple **acid phosphatases**. Homology models indicate that both **bacterial** proteins appear to be similar to mammalian purple **acid phosphatases** in the immediate vicinity of the active site. It is likely that these enzymes act as Fenton-type catalysts in order to prevent damage caused by reactive oxygen species generated by invaded host cells (M. tuberculosis) or by the light-harvesting complex (Synechocystis sp.). (C) 2000 Elsevier Science B.V. All rights reserved.

L38 ANSWER 30 OF 49 MEDLINE on STN DUPLICATE 12
 ACCESSION NUMBER: 2000122624 MEDLINE
 DOCUMENT NUMBER: PubMed ID: 10655611
 TITLE: **Crystal** structures of Escherichia coli phytase and its complex with phytate.
 AUTHOR: Lim D; Golovan S; Forsberg C W; Jia Z
 CORPORATE SOURCE: Department of Biochemistry, Queen's University, Kingston, Ontario K7L 3N6, Canada.
 SOURCE: Nature structural biology, (2000 Feb) 7 (2) 108-13. Journal code: 9421566. ISSN: 1072-8368.
 PUB. COUNTRY: United States
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 LANGUAGE: English

FILE SEGMENT: Priority Journals
OTHER SOURCE: PDB-1DKL; PDB-1DKM; PDB-1DKN; PDB-1DKO; PDB-1DKP; PDB-1DKQ
ENTRY MONTH: 200003
ENTRY DATE: Entered STN: 20000320
Last Updated on STN: 20000320
Entered Medline: 20000303

AB Phytases catalyze the hydrolysis of phytate and are able to improve the nutritional quality of phytate-rich diets. *Escherichia coli* phytase, a member of the histidine **acid phosphatase** family has the highest specific activity of all phytases characterized. The **crystal** structure of *E. coli* phytase has been determined by a two-wavelength anomalous diffraction method using the exceptionally strong anomalous scattering of tungsten. Despite a lack of sequence similarity, the structure closely resembles the overall fold of other histidine **acid phosphatases**. The structure of *E. coli* phytase in complex with phytate, the preferred substrate, reveals the binding mode and substrate recognition. The binding is also accompanied by conformational changes which suggest that substrate binding enhances catalysis by increasing the acidity of the general acid.

L38 ANSWER 31 OF 49 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
DUPLICATE 13

ACCESSION NUMBER: 2000:514265 BIOSIS
DOCUMENT NUMBER: PREV200000514265
TITLE: Site-directed mutagenesis improves catalytic efficiency and thermostability of *Escherichia coli* pH 2.5 **acid phosphatase**/phytase expressed in *Pichia pastoris*.
AUTHOR(S): Rodriguez, Eric; Wood, Zachary A.; Karplus, P. Andrew; Lei, Xin Gen [Reprint author]
CORPORATE SOURCE: Department of Animal Science, Cornell University, Ithaca, NY, 14853, USA
SOURCE: Archives of Biochemistry and Biophysics, (October 1, 2000) Vol. 382, No. 1, pp. 105-112. print.
CODEN: ABBIA4. ISSN: 0003-9861.
DOCUMENT TYPE: Article
LANGUAGE: English
OTHER SOURCE: Genbank-M58708
ENTRY DATE: Entered STN: 29 Nov 2000
Last Updated on STN: 12 Feb 2002

AB *Escherichia coli* pH 2.5 **acid phosphatase** gene (appA) and three mutants were expressed in *Pichia pastoris* to assess the effect of strategic mutations or deletion on the enzyme (EcAP) biochemical properties. Mutants A131N/V134N/D207N/S211N, C200N/D207N/S211N, and A131N/V134N/C200N/D207N/S211N had four, two, and four additional potential N-glycosylation sites, respectively. Extracellular phytase and **acid phosphatase** activities were produced by these mutants and the intact enzyme r-AppA. The N-glycosylation level was higher in mutants A131N/V134N/D207N/S211N (48%) and A131N/V134N/C200N/D207N/S211N (89%) than that in r-AppA (14%). Despite no enhancement of glycosylation, mutant C200N/D207N/S211N was different from r-AppA in the following properties. First, it was more active at pH 3.5-5.5. Second, it retained more ($P < 0.01$) phytase activity than that of r-AppA. Third, its specific activity of phytase was 54% higher. Lastly, its apparent catalytic efficiency k_{cat}/K_m for either p-nitrophenyl phosphate (5.8×10^5 vs $2.0 \times 10^5 \text{ min}^{-1} \text{ M}^{-1}$) or sodium phytate (6.9×10^6 vs $1.1 \times 10^6 \text{ min}^{-1} \text{ M}^{-1}$) was improved by factors of 1.9- and 5.3-fold, respectively. Based on the recently published *E. coli* phytase **crystal** structure, substitution of C200N in mutant C200N/D207N/S211N seems to eliminate the disulfide bond between the G helix and the GH loop in the alpha-domain of the protein. This change may modulate the domain flexibility and thereby the catalytic efficiency and thermostability of the enzyme.

L38 ANSWER 32 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN DUPLICATE 14

ACCESSION NUMBER: 1999:761694 CAPLUS
DOCUMENT NUMBER: 132:1481
TITLE: Structure, properties, and reactivity of the Fe(II)Fe(III) and Zn(II)Fe(III) purple **acid phosphatases**
AUTHOR(S): Twitchett, Mark B.; Sykes, A. Geoffrey
CORPORATE SOURCE: Dep. Chemistry, Univ. Newcastle, Newcastle upon Tyne,

SOURCE: NE1 7RU, UK
European Journal of Inorganic Chemistry (1999), (12),
2105-2115
CODEN: EJICFO; ISSN: 1434-1948
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB The review with 101 refs. describes the structure, properties, and mechanisms of the purple **acid phosphatases** (PAP). The enzyme is isolated from mammalian, plant and **bacterial** sources. **X-ray** structural information is now available for the enzyme from pig (uteroferrin), rat and kidney beans. Features of the mechanism are the concerted action of a labile M(II) center (Fe(II) or Zn(II)) alongside a more inert Fe(III). The latter is effective as a conjugate-base FeOH2+, which initiates hydrolysis at the M(II)-bound phosphate ester by a process involving OH- replacement of OR- at the P(V). His residues near to the active site help bind the phosphate and are involved in the release of OR-. Effects of replacement of the Fe(II) by Mn(II), Co(II), Ni(II), Cu(II), and Zn(II), and of Fe(III) by Ga(III), Al(III), and In(III) have been studied. The mechanistic role of the Zn(II)Zn(II) combination in alk. **phosphatases**, and other related dinuclear centers is also considered.

REFERENCE COUNT: 101 THERE ARE 101 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 33 OF 49 SCISEARCH COPYRIGHT 2004 THOMSON ISI on STN

ACCESSION NUMBER: 1999:233599 SCISEARCH

THE GENUINE ARTICLE: 177MW

TITLE: Preliminary **X-ray** crystallographic analysis of a novel phytase from a Bacillus amyloliquefaciens strain

AUTHOR: Ha N C; Kim Y O; Oh T K; Oh B H (Reprint)

CORPORATE SOURCE: POHANG UNIV SCI & TECHNOL, DEPT LIFE SCI, POHANG 790784, KYUNGBUK, SOUTH KOREA (Reprint); POHANG UNIV SCI & TECHNOL, DEPT LIFE SCI, POHANG 790784, KYUNGBUK, SOUTH KOREA; POHANG UNIV SCI & TECHNOL, SCH ENVIRONM ENGN, POHANG 790784, KYUNGBUK, SOUTH KOREA; KOREA RES INST BIOSCI & BIOTECHNOL, MICROBIAL ENZYME RU, TAEJON 305600, SOUTH KOREA

COUNTRY OF AUTHOR: SOUTH KOREA

SOURCE: ACTA CRYSTALLOGRAPHICA SECTION D-BIOLOGICAL CRYSTALLOGRAPHY, (MAR 1999) Vol. 55, Part 3, pp. 691-693. Publisher: MUNKSGAARD INT PUBL LTD, 35 NORRE SOGADE, PO BOX 2148, DK-1016 COPENHAGEN, DENMARK. ISSN: 0907-4449.

DOCUMENT TYPE: Article; Journal

FILE SEGMENT: LIFE

LANGUAGE: English

REFERENCE COUNT: 21

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB A novel **bacterial** phytase from a Bacillus amyloliquefaciens strain was crystallized using the hanging-drop vapour-diffusion method. The amino-acid sequence of the enzyme does not show any homology to those of other known phytases or **phosphatases**, with the exception of a phytase from Bacillus subtilis. The enzyme exhibits a thermal stability which is strongly dependent on calcium ions. High-quality single **crystals** of the enzyme in the absence of calcium ions were obtained using a precipitant solution containing 20% 2-methyl-2,4-pentanediol and 0.1 M MES (pH 6.5). Native diffraction data to 2.0 Angstrom resolution were obtained from a flash-frozen **crystal** at 110 K using a rotating-anode **X-ray** source. The **crystals** belong to space group P2(1)2(1)2(1) with unit-cell dimensions a = 50.4, b = 64.1, c = 104.2 Angstrom and contain one monomer per asymmetric unit. Structure determination using heavy-atom derivative **crystals** is in progress, along with an effort to crystallize the calcium ion bound form of the enzyme.

L38 ANSWER 34 OF 49 MEDLINE on STN

DUPLICATE 15

ACCESSION NUMBER: 1999242008 MEDLINE

DOCUMENT NUMBER: PubMed ID: 10227469

TITLE: Hydrolytic and enzymatic incubation of polyhydroxyoctanoate (PHO): a short-term in vitro study of a degradable **bacterial** polyester.

AUTHOR: Marois Y; Zhang Z; Vert M; Deng X; Lenz R; Guidoin R

CORPORATE SOURCE: CRBA-URA CNRS 1465, Faculte de Pharmacie, Universite de Montpellier I, France.

SOURCE: Journal of biomaterials science. Polymer edition, (1999) 10 (4) 483-99.
Journal code: 9007393. ISSN: 0920-5063.

PUB. COUNTRY: Netherlands

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

FILE SEGMENT: Priority Journals

ENTRY MONTH: 199906

ENTRY DATE: Entered STN: 19990618
Last Updated on STN: 19990618
Entered Medline: 19990607

AB The present study examined the degradation behaviour of poly(beta-hydroxy octanoate) (PHO), a **bacterial** poly(beta-hydroxy alcanoate), following incubation under hydrolytic or enzymatic conditions in vitro. Solution-cast PHO films were incubated in a citrate buffer solution with and without **acid phosphatase** and in an acetate buffer with and without beta-glucuronidase for periods ranging from 7 to 60 days. The physical characterization of the PHO films was analyzed by SEM and tensile strength studies. In addition, various analytical methods were used to detect modifications in the chemical and morphological structure of the PHO, namely, ESCA, FTIR, DSC, **X-ray** diffraction, and SEC. The results indicate that the enzymatic conditions selected in the present study induced no significant surface morphological or chemical modifications, and no significant weight loss was observed after 60 days of incubation. However, as revealed by weight average molecular weight Mw and number average molecular weight Mn decreases, changes in the bulk structure of the PHO were observed with **acid phosphatase** at 28 and 60 days, in contrast to smaller Mw and Mn decreases recorded in both the buffers and the beta-glucuronidase. The tensile properties had decreased following incubation, yet showed no difference under all of the selected conditions. With no weight loss or surface changes, the PHO films incubated in **acid phosphatase** showed only a chemical hydrolytic process characterized by Mw and Mn decreases with time of incubation. The present study demonstrated that the degradation of PHO films is one of slow, chemical hydrolysis only, perhaps requiring several months of incubation. The hydrophobic nature of the long alkyl pendent chain in PHO may be responsible for this slow process. The inability of enzymes to degrade PHO may be attributed to the latter's poor adsorption capacity, due to its hydrophobic nature, and to a lack of specificity in the catalytic activity of these enzymes.

L38 ANSWER 35 OF 49 SCISEARCH COPYRIGHT 2004 THOMSON ISI on STN

ACCESSION NUMBER: 1999:439807 SCISEARCH

THE GENUINE ARTICLE: 203AJ

TITLE: A novel isoform of the low molecular weight phosphotyrosine **phosphatase**, LMTP-C, arising from alternative mRNA splicing

AUTHOR: Tailor P; Gilman J; Williams S; Mustelin T (Reprint)

CORPORATE SOURCE: SIDNEY KIMMEL CANC CTR, LAB SIGNAL TRANSDUCT, 10835 ALTMAN ROW, SAN DIEGO, CA 92121 (Reprint); LA JOLLA INST ALLERGY & IMMUNOL, DIV CELL BIOL, SAN DIEGO, CA

COUNTRY OF AUTHOR: USA

SOURCE: EUROPEAN JOURNAL OF BIOCHEMISTRY, (JUN 1999) Vol. 262, No. 2, pp. 277-282.
Publisher: BLACKWELL SCIENCE LTD, P O BOX 88, OSNEY MEAD, OXFORD OX2 ONE, OXON, ENGLAND.
ISSN: 0014-2956.

DOCUMENT TYPE: Article; Journal

FILE SEGMENT: LIFE

LANGUAGE: English

REFERENCE COUNT: 24

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB The low molecular weight protein tyrosine **phosphatase** (LMTPC) is an 18-kDa enzyme that is distantly related to other protein tyrosine

phosphatases. The single gene for LMPTP is known to undergo an alternative splicing event in which exon 3 or exon 4 is excised, resulting in two isoforms termed A and B; the latter is more mobile in SDS/PAGE. In this paper we report the existence of a third isoform, which we call C, in which both exons 3 and 4 are lacking. We find the resulting mRNA to be ubiquitously expressed at levels that exceed those of the mRNAs for isoforms A and B. This mRNA was reverse-transcribed, cloned and sequenced, confirming the direct splicing of exon 2 to exon 5. In-vitro transcription and translation of the cDNA for the novel isoform resulted in the expected 16 kDa protein. This protein was also detected in Jurkat T cells using an antipeptide antiserum. LMPTP-C immunoprecipitated from transfected cells, as well as **bacterially** produced recombinant LMPTP-C, lacked **phosphatase** activity. Unlike LMPTP-B, LMPTP-C was not phosphorylated on tyrosine when coexpressed with Lck despite the presence of the two acceptor tyrosines. Finally, whereas c-fas induction by platelet-derived growth factor was inhibited by LMPTP-B, LMPTP-C augmented it. These results suggest that the lack of the 38-amino acid fragment encoded by exon 3 or 4 results in a protein product with a different three-dimensional folding, that lacks a functional catalytic pocket and that may function as a natural antagonist of isoforms A and B.

L38 ANSWER 36 OF 49 SCISEARCH COPYRIGHT 2004 THOMSON ISI on STN

ACCESSION NUMBER: 1998:609395 SCISEARCH

THE GENUINE ARTICLE: 107NW

TITLE: The Escherichia coli chaperonin 60 (groEL) is a potent stimulator of osteoclast formation

AUTHOR: Reddi K; Meghji S; Nair S P; Arnett T R; Miller A D; Preuss M; Wilson M; Henderson B (Reprint); Hill P

CORPORATE SOURCE: UNIV COLL LONDON, EASTMAN DENT INST, MAXILLOFACIAL SURG RES UNIT, 256 GRAYS INN RD, LONDON WC1X 8LD, ENGLAND (Reprint); UNIV COLL LONDON, EASTMAN DENT INST, MAXILLOFACIAL SURG RES UNIT, LONDON WC1X 8LD, ENGLAND; UNIV COLL LONDON, DEPT ANAT & DEV BIOL, LONDON WC1X 8LD, ENGLAND; UNIV COLL LONDON, EASTMAN DENT INST, DEPT MICROBIOL, LONDON WC1X 8LD, ENGLAND; UNIV LONDON IMPERIAL COLL SCI TECHNOL & MED, DEPT CHEM, LONDON, ENGLAND; UNITED MED & DENT SCH GUYS & ST THOMAS HOSP, DEPT ORTHODONT & PAEDIAT DENT, LONDON SE1 9RT, ENGLAND

COUNTRY OF AUTHOR: ENGLAND

SOURCE: JOURNAL OF BONE AND MINERAL RESEARCH, (AUG 1998) Vol. 13, No. 8, pp. 1260-1266. Publisher: BLACKWELL SCIENCE INC, 350 MAIN ST, MALDEN, MA 02148.

ISSN: 0884-0431.

DOCUMENT TYPE: Article; Journal

FILE SEGMENT: LIFE

LANGUAGE: English

REFERENCE COUNT: 33

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB Chaperonins (cpns) are intracellular oligomeric protein complexes that fold and refold proteins in a catalytic manner and aid in the transmembrane transport of cellular proteins. We reported previously that the lipopolysaccharide-free recombinant cpn60 of Escherichia coli (groEL) is able to stimulate the breakdown of murine calvarial bone in culture and showed that such resorption is potentially inhibited by an inhibitor of the enzyme cyclo-oxygenase and to a lesser extent by inhibitors of 5-lipoxygenase. In this study, we have investigated the effects of groEL on the resorptive activity and formation of osteoclasts in culture. In low density, osteoclast-containing cultures from neonatal rats incubated for 24 or 96 h on dentine discs, groEL (1-1000 ng/ml) stimulated resorption pit formation up to 4-fold, but this effect, was essentially dependent on cell number. Using 12-day cultures of mouse bone marrow to assess osteoclast recruitment, groEL (1-1000 ng/ml) caused a dramatic dose-dependent stimulation of the formation of tartrate-resistant **acid phosphatase**-positive multinucleated cells and the resorption of the dentine on which bone marrow cells were cultured. Osteoclast formation elicited by groEL was almost completely abolished by indomethacin, an inhibitor of cyclo-oxygenase, but was unaffected by inhibitors of 5-lipoxygenase, suggesting that prostaglandins but not leukotrienes may mediate the action of groEL on osteoclastogenesis. It is possible that **bacterial** cpn60s such as groEL may play a role in

the osteolysis associated with bone infections. Whether endogenous ('self') chaperonins have a role in other bone loss disorders, such as osteoporosis, is an intriguing possibility.

L38 ANSWER 37 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:778021 CAPLUS
DOCUMENT NUMBER: 130:121174
TITLE: Vanadate-containing haloperoxidases and **acid phosphatases**: the conserved active site
AUTHOR(S): Hemrika, Wieger; Renirie, Rokus; Dekker, Henk; Wever, Ron
CORPORATE SOURCE: E. C. Slater Institute, University of Amsterdam, Amsterdam, 1018 TV, Neth.
SOURCE: ACS Symposium Series (1998), 711(Vanadium Compounds), 216-227
CODEN: ACSMC8; ISSN: 0097-6156
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review with 40 refs. We have shown that the amino acid residues contributing to the active site of vanadate-contg. chloroperoxidase from the fungus *Curvularia inaequalis*, of which the **crystal** structure is known, are conserved within a large and diverse group of **acid phosphatases**, that include amongst others **bacterial acid phosphatases**, mammalian glucose-6-phosphatases and type 2 phosphatidic **acid phosphatases**. The suggestion that the active sites of these enzymes are structurally similar is confirmed by activity measurements showing that apochloroperoxidase exhibits **phosphatase** activity. These observations not only reveal interesting evolutionary relationships between these groups of enzymes but also have important implications for the research on **acid phosphatases** since structural data are lacking for this group of enzymes. Based on the conservation of the active sites we propose a new membrane topol. model for glucose-6-phosphatase.

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L38 ANSWER 38 OF 49 MEDLINE on STN DUPLICATE 16

ACCESSION NUMBER: 97194074 MEDLINE
DOCUMENT NUMBER: PubMed ID: 9041652
TITLE: Identification of a novel **phosphatase** sequence motif.
AUTHOR: Stukey J; Carman G M
CORPORATE SOURCE: Department of Biology, Hope College, Holland, Michigan 49422, USA.. stukey@hope.edu
CONTRACT NUMBER: GM-28140 (NIGMS)
SOURCE: Protein science : a publication of the Protein Society, (1997 Feb) 6 (2) 469-72.
Journal code: 9211750. ISSN: 0961-8368.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199706
ENTRY DATE: Entered STN: 19970612
Last Updated on STN: 19970612
Entered Medline: 19970603

AB We have identified a novel, conserved **phosphatase** sequence motif, KXXXXXXRP-(X12-54)-PSGH-(X31-54)-SRXXXXX HXXXX, that is shared among several lipid **phosphatases**, the mammalian glucose-6-phosphatases, and a collection of **bacterial** nonspecific **acid phosphatases**. This sequence was also found in the vanadium-containing chloroperoxidase of *Curvularia inaequalis*. Several lines of evidence support this **phosphatase** motif identification. **Crystal** structure data on chloroperoxidase revealed that all three domains are in close proximity and several of the conserved residues are involved in the binding of the cofactor, vanadate, a compound structurally similar to phosphate. Structure-function analysis of the human glucose-6-phosphatase has shown that two of the conserved residues (the first domain arginine and the central domain histidine) are essential for

enzyme activity. This conserved sequence motif was used to identify nine additional putative **phosphatases** from sequence databases, one of which has been determined to be a lipid **phosphatase** in yeast.

L38 ANSWER 39 OF 49 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
ACCESSION NUMBER: 1997:64051 BIOSIS
DOCUMENT NUMBER: PREV199799363254
TITLE: Deglycosylation of proteins for crystallization using recombinant fusion protein glycosidases.
AUTHOR(S): Grueninger-Leitch, Fiona [Reprint author]; D'Arcy, Allan; D'Arcy, Brigitte; Chene, Christiane
CORPORATE SOURCE: Dep. Gene Technol., Pharma Preclinical Res., F. Hoffmann-La Roche AG, CH-4070 Basel, Switzerland
SOURCE: Protein Science, (1996) Vol. 5, No. 12, pp. 2617-2622.
ISSN: 0961-8368.
DOCUMENT TYPE: Article
LANGUAGE: English
ENTRY DATE: Entered STN: 11 Feb 1997
Last Updated on STN: 11 Feb 1997

AB Obtaining high quality protein **crystals** remains a rate-limiting step in the determination of three-dimensional **X-ray** structures. A frequently encountered problem in this respect is the high or heterogeneous carbohydrate content of many eukaryotic proteins. A number of reports have demonstrated the use of enzymatic deglycosylation in the crystallization of certain glycoproteins. Although this is an attractive tool, there are some problems that hinder the more widespread use of glycosidases in crystallization. First, commercially available glycosidases are relatively expensive, which virtually prohibits their use on a large scale. Second, the glycosidase must be removed from the glycoprotein of interest following deglycosylation, which is not always straightforward. To circumvent these problems we have cloned the two most generally useful glycosidases, peptide-N-glycosidase F and endoglycosidase F-1 from *Flavobacterium meningosepticum*, as fusion proteins with glutathione S-transferase. The fusion not only allows rapid purification of these enzymes from *Escherichia coli* cell extracts, but also permits rapid removal from target proteins following deglycosylation. We have used these enzymes to obtain **crystals** of phytase from *Aspergillus ficuum* and **acid phosphatase** from *Aspergillus niger* and to obtain a new **crystal** form of recombinant human renin.

L38 ANSWER 40 OF 49 MEDLINE on STN DUPLICATE 17
ACCESSION NUMBER: 95034702 MEDLINE
DOCUMENT NUMBER: PubMed ID: 7947683
TITLE: Resonance Raman evidence for an Fe-O-Fe center in stearoyl-ACP desaturase. Primary sequence identity with other diiron-oxo proteins.
AUTHOR: Fox B G; Shanklin J; Ai J; Loehr T M; Sanders-Loehr J
CORPORATE SOURCE: Institute for Enzyme Research, Graduate School, University of Wisconsin, Madison 53705.
CONTRACT NUMBER: GM-18865 (NIGMS)
SOURCE: Biochemistry, (1994 Nov 1) 33 (43) 12776-86.
Journal code: 0370623. ISSN: 0006-2960.
PUB. COUNTRY: United States
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199412
ENTRY DATE: Entered STN: 19950110
Last Updated on STN: 19970203
Entered Medline: 19941201

AB The stearoyl-ACP delta 9 desaturase from plants is a new example of a growing number of proteins that contain oxo- or hydroxo-bridged diiron clusters. On the basis of differences in primary sequence motifs providing the cluster ligands and upon structural differences elucidated by **X-ray** crystallography, we now propose that the presently known, soluble diiron-oxo proteins can be grouped into two classes, I and II. Class I contains hemerythrin, myohemerythrin, and, possibly, purple **acid phosphatase**. Class II contains ribonucleotide reductases, **bacterial** hydrocarbon hydroxylases (methane monooxygenase, toluene-4-monooxygenase, and phenol hydroxylase),

rubrerythrin, and stearyl-ACP desaturases. Through the use of resonance Raman spectroscopy, we have detected symmetric ($\nu_s = 519 \text{ cm}^{-1}$) and asymmetric ($\nu_{as} = 747 \text{ cm}^{-1}$) vibrational modes in the castor stearyl-ACP delta 9 desaturase, which are typical of oxo-bridged diiron clusters. These frequencies shift by -18 and -34 cm^{-1} , respectively, in H218O, proving that the bridging ligand is readily exchangeable with solvent ($t_{1/2} = 7 \text{ min}$). Calculation of an approximately 123° Fe-O-Fe angle from the position of ν_s and ν_{as} and from the ^{18}O -dependent shift in these frequencies suggests that the diiron-oxo cluster in the desaturase is triply bridged in the diferric state. In the diferrous state, the two iron sites of the cluster are structurally inequivalent, as shown by differential temperature dependence of the Mossbauer quadrupole splittings. For the class II diiron-oxo proteins, primary sequence alignments reveal conserved amino acid residues which act as iron cluster ligands, participate in a hydrogen-bonding network, and are potentially involved in O_2 binding and activation. Based on this conservation, a structural model for the stearyl-ACP delta 9 desaturase active site is proposed that has strong similarity to both ribonucleotide reductase and methane monooxygenase. However, after single turnover of the diferous state with $^{18}\text{O}_2$, ^{18}O is not detected in the oxo bridge of the castor desaturase. This is in contrast to the outcome observed for ribonucleotide reductase, suggesting the desaturase and ribonucleotide reductase differ in certain aspects of their respective O_2 -activation reactions.

L38 ANSWER 41 OF 49 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
 ACCESSION NUMBER: 1993:387022 BIOSIS
 DOCUMENT NUMBER: PREV199396062322
 TITLE: EXAFS studies of uteroferrin and its anion complexes.
 AUTHOR(S): True, Anne E.; Scarrow, Robert C.; Randall, Clayton R.; Holz, Richard C.; Que, Lawrence, Jr. [Reprint author]
 CORPORATE SOURCE: Dep Chem., University Minnesota, Minneapolis, MN 55455, USA
 SOURCE: Journal of the American Chemical Society, (1993) Vol. 115, No. 10, pp. 4246-4255.
 CODEN: JACSAT. ISSN: 0002-7863.
 DOCUMENT TYPE: Article
 LANGUAGE: English
 ENTRY DATE: Entered STN: 23 Aug 1993
 Last Updated on STN: 28 Sep 1993

AB Iron K-edge X-ray absorption data on the purple acid phosphatase from porcine uterus (uteroferrin, Uf) have been obtained for the native reduced enzyme and for the oxidized enzyme in its phosphate- and arsenate-bound forms. In all three complexes, the first sphere consists of 1.5 N/O at approx 1.94 \AA , 4 N/O at approx 2.1 \AA , and 0.5-1 N/O at approx 2.4 \AA ; in no complex is found an Fe-O bond of approx 1.8 \AA which would derive from a μ -oxo-bond. The approx 1.94 \AA shell corresponds to Fe-OAr and Fe- μ -OH(or R) bonds. The approx $2.1\text{-}\text{ \AA}$ shell arises from histidine, carboxylate, oxoanion, and solvent ligation. The scatterer at approx 2.4 \AA is associated with a chelated carboxylate residue. The second-sphere analysis for Uf-r indicates an Fe-Fe distance of 3.52 \AA , similar to those found for semimethemerythrin azide, methane monooxygenase, and related model complexes, which suggests the presence of a (μ -hydroxo or alkoxo)diiron unit supported by a carboxylate bridge. On the basis of the EXAFS analysis and other spectroscopic data, it is proposed that tyrosine and histidine are terminal ligands to the Fe(III) center, and histidine and the chelated carboxylate coordinate to the Fe(II) center, with solvent molecules completing the diiron coordination sphere. This proposed active site is slightly modified from that found for the R2 protein of ribonucleotide reductase from Escherichia coli and suggested for the hydroxylase component of methane monooxygenase. The diiron cores of Uf-O cntdot PO-4 and Uf-O cntdot AsO-4 are significantly different from that of Uf-r. Given the absence of a 1.8 \AA bond, the diferric sites are not oxo-bridged, a conclusion also corroborated by the small intensity of the $1s \rightarrow 3d$ preedge features in these complexes. The Fe-Fe distances of approx $3.2\text{-}3.3 \text{ \AA}$ found for Uf-O cntdot PO-4 and Uf-O cntdot AsO-4 must then arise from an Fe-2(OR)-2 core. The observed Fe-P (3.17 \AA) and Fe-As (3.41 \AA) distances correspond to Fe-O-P(As) angles indicative of a bidentate bridging oxoanion which supports the Fe-2O-2 core.

L38 ANSWER 42 OF 49 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: 1993:387023 BIOSIS
DOCUMENT NUMBER: PREV199396062323
TITLE: Direct observation of the push effect on the O-O bond cleavage of acylperoxoiron(III) porphyrin complexes.
AUTHOR(S): Yamaguchi, Kazuya; Watanabe, Yoshihito [Reprint author]; Morishima, Isao [Reprint author]
CORPORATE SOURCE: Div. Mol. Engineering, Graduate Sch. Engineering, Kyoto University, Kyoto 606-01, Japan
SOURCE: Journal of the American Chemical Society, (1993) Vol. 115, No. 10, pp. 4058-4065.
CODEN: JACSAT. ISSN: 0002-7863.
DOCUMENT TYPE: Article
LANGUAGE: English
ENTRY DATE: Entered STN: 23 Aug 1993
Last Updated on STN: 28 Sep 1993

AB The first direct observation of the push effect on heterolytic and homolytic O-O bond cleavage steps of acylperoxoiron(III) porphyrin complexes is reported for a series of acylperoxoiron(III) porphyrins (5) having substituents at the meso-positions of the porphyrin ring. Transformation of 5 to the corresponding oxoferry (O dbd Fe-IV) porphyrin cation radicals (6) in methylene chloride at -80 degree C by heterolytic O-O bond cleavage was found to be first order in (5). Introduction of electron-donating substituents at the meso-positions of the porphyrins ring facilitates the O-O bond cleavage in 5. Addition of 1 equiv of imidazole derivatives to a methylene chloride solution of 5 immediately gave an acylperoxoiron(III) porphyrin-imidazole adduct (9). The conversion of 9 to 6 was also found to be first order in (9), and the coordination of electron-rich imidazole derivatives strongly encouraged the O-O bond cleavage of 9. On the other hand, the push effect on the homolytic O-O bond cleavage reaction has been examined in toluene at -6 degree C to about -40 degree C. The homolytic O-O bond cleavage of 9 afforded the imidazole adduct of oxoferryl porphyrin complex 7 when phenylperacetic acid was employed. Homolysis of the O-O bond is enhanced by the imidazole ligation; however, the push effect on homolysis is much less than that on heterolysis. These results explain the biological utilization of strong electron-donor ligands in heme enzymes such as peroxidase, cytochrome P-450, and catalase.

L38 ANSWER 43 OF 49 SCISEARCH COPYRIGHT 2004 THOMSON ISI on STN

ACCESSION NUMBER: 92:520349 SCISEARCH
THE GENUINE ARTICLE: JK900
TITLE: BINUCLEAR IRON CENTERS IN PROTEINS
AUTHOR: WILKINS R G (Reprint)
CORPORATE SOURCE: UNIV WARWICK, DEPT CHEM, COVENTRY CV4 7AL, W MIDLANDS, ENGLAND (Reprint)
COUNTRY OF AUTHOR: ENGLAND
SOURCE: CHEMICAL SOCIETY REVIEWS, (SEP 1992) Vol. 21, No. 3, pp. 171-178.
ISSN: 0306-0012.
DOCUMENT TYPE: General Review; Journal
FILE SEGMENT: PHYS
LANGUAGE: ENGLISH
REFERENCE COUNT: 47

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB Binuclear iron sites with bridging ligands feature in a number of important non-haem iron proteins. Haemerythrin is the respiratory protein in marine worms. In addition, there are the enzymes ribonucleotide reductase, important in DNA synthesis; purple **acid phosphatases** with as yet unknown function; and methane monooxygenase, from methanotropic **bacteria**, which catalyses the insertion of O into C-H bonds. The variety of techniques used in their structural characterization is described from an historical viewpoint. Finally, the reactivity and mechanisms of action of these proteins are briefly discussed.

L38 ANSWER 44 OF 49 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: 1986:231112 BIOSIS
DOCUMENT NUMBER: PREV198630113608; BR30:113608
TITLE: COMPARATIVE STUDIES ON MATRIX VESICLES IN RAT BONE AFTER LOCAL AND SYSTEMIC INJURIES.
AUTHOR(S): SELA J [Reprint author]

CORPORATE SOURCE: ORAL PATHOLOGY HEBREW UNIVERSITY, HADASSAH SCHOOL DENTAL
MEDICINE, JERUSALEM, ISRAEL
SOURCE: Bone (New York), (1985) Vol. 6, No. 6, pp. 478.
Meeting Info.: SYMPOSIUM ON CELL-MEDIATED CALCIFICATION AND
MATRIX VESICLES HELD AT THE IV INTERNATIONAL CONFERENCE ON
MATRIX VESICLES, CAMBRIDGE, ENGLAND, JULY 1-5, 1985. BONE
(N Y).
CODEN: BONEDL. ISSN: 8756-3282.
DOCUMENT TYPE: Conference; (Meeting)
FILE SEGMENT: BR
LANGUAGE: ENGLISH
ENTRY DATE: Entered STN: 1 Jun 1986
Last Updated on STN: 1 Jun 1986

L38 ANSWER 45 OF 49 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
ACCESSION NUMBER: 1980:235593 BIOSIS
DOCUMENT NUMBER: PREV198070028089; BA70:28089
TITLE: SUCCESSFUL BONE MARROW TRANSPLANTATION FOR INFANTILE
MALIGNANT OSTEOPETROSIS.
AUTHOR(S): COCCIA P F [Reprint author]; KRIVIT W; CERVENKA J; CLAWSON
C; KERSEY J H; KIM T H; NESBIT M E; RAMSAY N K C; WARKENTIN
P I
CORPORATE SOURCE: BOX 228, MAYO MEML BUILD, UNIV MINN HEALTH SCI CENT,
MINNEAPOLIS, MINN 55455, USA
SOURCE: New England Journal of Medicine, (1980) Vol. 302, No. 13,
pp. 701-708.
CODEN: NEJMAG. ISSN: 0028-4793.
DOCUMENT TYPE: Article
FILE SEGMENT: BA
LANGUAGE: ENGLISH

AB A 5-mo.-old girl with autosomal-recessive osteopetrosis received a bone
marrow transplant from her 5-yr-old HLA-MLC[mixed lymphocyte
culture]-identical brother after preparation with cyclophosphamide and
modified total-body irradiation. Engraftment was documented by
chromosomal analysis. Anemia, thrombocytopenia and leukoerythroblastosis
corrected within 12 wk of transplantation. Low serum Ca and elevated
serum alkaline and **acid phosphatase** levels became
normal. Serial **X-ray** studies revealed bony remodeling
and new nonsclerotic bone formation. A pretransplantation bone biopsy
revealed small marrow spaces, rare marrow elements, increased osteoclasts
and no bony resorption. After transplantation, osteoclasts were actively
resorbing bone, and medullary cavities contained normal bone marrow.
Fluorescent Y-body analysis after transplantation revealed donor (male)
osteoclasts and recipient (female) osteoblasts. Monocyte bactericidal
activity, markedly decreased before transplantation, became normal.
Vision, hearing, growth and development were progressively improving 16
mo. after transplantation. Allogeneic bone marrow transplantation appears
to be the treatment of choice in this fatal disorder.

L38 ANSWER 46 OF 49 EMBASE COPYRIGHT 2004 ELSEVIER INC. ALL RIGHTS RESERVED.
on STN
ACCESSION NUMBER: 76063442 EMBASE
DOCUMENT NUMBER: 1976063442
TITLE: Induction of autophagic vacuoles in peritoneal cells.
AUTHOR: Komiyama A.; Spicer S.S.; Bank H.; Farrington J.
CORPORATE SOURCE: United States
SOURCE: RES Journal of the Reticuloendothelial Society, (1975) 17/3
(146-161).
CODEN: RESJAS
DOCUMENT TYPE: Journal
FILE SEGMENT: 026 Immunology, Serology and Transplantation
025 Hematology
005 General Pathology and Pathological Anatomy
LANGUAGE: English

AB Rat peritoneal macrophages developed inclusions interpreted as autophagic
vacuoles after peritoneal infusion of phosphate buffered saline (PBS) with
or without colloidal gold. These infusions were absent 5 min, but quite
numerous 15 to 30 min, after injection. The early inclusions were
continuous with and apparently derived from the nuclear envelope,
sequestered normal appearing cytoplasmic areas, had little **acid
phosphatase** activity and contained no endocytosed gold. At 45 to

60 min post injection, most of these autophagic vacuoles lay free in the cytoplasm, were delimited by a thick membrane like that of heterophagic bodies and appeared involuted, containing heterogenous material, myelin figures and abundant **acid phosphatase**. Such late vacuoles containing sparse gold particles constituted autoheterophagosomes. Macrophages had few autophagic vacuoles after peritoneal infusion of fetal calf serum (FCS) or tissue culture medium. However, macrophages harvested 45 to 60 min following injection of FCS revealed lucent **crystals** in their heterophagic bodies. Microendocytic vesicles appeared to bud from the subsurface vacuole like profiles that were often located at one pole of the cell. These vesicles endocytosed gold particles and transported them to the numerous heterophagic dense bodies (microendosomes) in macrophages. These heterophagic bodies resulting from microendocytosis differed in structure and more active gold uptake from **bacteria** laden, phagocytic vacuoles characteristic of macroendocytosis. Both the latter macroendosomes and the microendosomes evidenced **acid phosphatase** indicative of secondary lysosomes but often differed in gold content and apparently remained discrete. Eosinophils, lymphocytes and mast cells developed fewer autophagic vacuoles and endocytosed fewer fold particles than did macrophages.

L38 ANSWER 47 OF 49 MEDLINE on STN DUPLICATE 18
 ACCESSION NUMBER: 76064839 MEDLINE
 DOCUMENT NUMBER: PubMed ID: 4468857
 TITLE: Effect of X-irradiation on various functions of murine macrophages.
 AUTHOR: Geiger B; Gallily R
 SOURCE: Clinical and experimental immunology, (1974 Apr) 16 (4) 643-55.
 Journal code: 0057202. ISSN: 0009-9104.
 PUB. COUNTRY: ENGLAND: United Kingdom
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals
 ENTRY MONTH: 197602
 ENTRY DATE: Entered STN: 19900313
 Last Updated on STN: 19900313
 Entered Medline: 19760227

L38 ANSWER 48 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1969:9448 CAPLUS
 DOCUMENT NUMBER: 70:9448
 TITLE: Staphylococcus **acid phosphatase**
 AUTHOR(S): Hadama, Yukinobu
 CORPORATE SOURCE: Kyoto Pref. Univ. Med., Kyoto, Japan
 SOURCE: Chemotherapy (Tokyo) (1968), 16(3), 349-58
 CODEN: NKRZAZ; ISSN: 0009-3165
 DOCUMENT TYPE: Journal
 LANGUAGE: Japanese

AB About 100 strains of staphylococci were isolated from patients and **acid phosphatase** activity and some other activities were measured. A modified p-nitrophenylphosphate method was established for **acid phosphatase** measurement in Staphylococcus. The relation of **acid phosphatase** activity to pathogenicity or virulence was also examd. Coagulase activity correlated well with **acid phosphatase** activity. A correlation was also found between **acid phosphatase** activity and pathogenicity or inductivity of intracutaneous reaction in mice. Strains with high **acid phosphatase** activity had potent mannose-decomp. and hemolytic activities. Strains of 80/81 phage type produced more **acid phosphatase** than those of other phage types. Strains with high **acid phosphatase** activity formed light blue or yellow colonies on **crystal** violet media, while those with low activity formed white colonies.

L38 ANSWER 49 OF 49 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 1959:113998 CAPLUS
 DOCUMENT NUMBER: 53:113998
 ORIGINAL REFERENCE NO.: 53:20472h-i,20473a-b
 TITLE: Histological and histochemical changes in temporary

AUTHOR(S): moniodoacetate mange
 BRAUN-FALCO, O.; THEISEN, H.
 CORPORATE SOURCE: Johannes-Gutenberg Univ., Mainz, Germany
 SOURCE: Arch. klin. u. exptl. Dermatol. (1959), 208, 539-58
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

AB Intracutaneous injection of 0.5 ml. of 0.01M CH₂ICOOH in 0.1M Na₂HPO₄ buffer at pH 6 in rats produced a temporary reversible mange-like effect in the area of the injection. The mitotically active matrix cells of rat hairs, and all the remaining follicle structures are made sensitive by the enzyme inhibitor, and respond with a change in regeneration of hair follicles. Histochem. studies showed an initial decrease in succinic dehydrogenase activity presumably due to inhibition of the sulfhydryl groups of the enzyme by the iodoacetate. After 14 days the enzyme activity had returned to the normal level. **Acid phosphatase** was increased, in agreement with the increased production of nucleic acids. No increase in glycogen could be observed in the bulb cells, in contrast to the observed increase after **x-ray** exposure. It is suggested that administration of enzyme inhibitors produces a general effect similar to that of **x-rays** or **bacterial** infection. Thus the so-called dysfermentation of the active hair matrix is very important in reversible mange. The interruption in normal cellular metabolism or the presence and accumulation of abnormal metabolic products is suggested as being the direct cause of the hair falling.

=> s nucleoside and (phosphatase or kinase or phosphotransferase)

L39 4640 FILE MEDLINE
 L40 5640 FILE CAPLUS
 L41 3318 FILE SCISEARCH
 L42 1081 FILE LIFESCI
 L43 4329 FILE BIOSIS
 L44 3308 FILE EMBASE

TOTAL FOR ALL FILES

L45 22316 NUCLEOSIDE AND (PHOSPHATASE OR KINASE OR PHOSPHOTRANSFERASE)

=> s 145 and bacteria?

L46 339 FILE MEDLINE
 L47 299 FILE CAPLUS
 L48 161 FILE SCISEARCH
 L49 62 FILE LIFESCI
 L50 589 FILE BIOSIS
 L51 173 FILE EMBASE

TOTAL FOR ALL FILES

L52 1623 L45 AND BACTERIA?

=> s 152 not 138

L53 13 S L38
 L54 339 FILE MEDLINE
 L55 6 S L38
 L56 298 FILE CAPLUS
 L57 17 S L38
 L58 161 FILE SCISEARCH
 L59 0 S L38
 L60 62 FILE LIFESCI
 L61 12 S L38
 L62 588 FILE BIOSIS
 L63 1 S L38
 L64 173 FILE EMBASE

TOTAL FOR ALL FILES

L65 1621 L52 NOT L38

=> s 165 not 2001-2004/py

L66 266 FILE MEDLINE
 L67 218 FILE CAPLUS
 L68 97 FILE SCISEARCH
 L69 39 FILE LIFESCI

L70 471 FILE BIOSIS
L71 113 FILE EMBASE

TOTAL FOR ALL FILES

L72 1204 L65 NOT 2001-2004/PY

=> s l72 and (x-ray or three dimension structure or x-ray)

L73 9 FILE MEDLINE
L74 5 FILE CAPLUS
L75 6 FILE SCISEARCH
L76 3 FILE LIFESCI
L77 21 FILE BIOSIS
L78 6 FILE EMBASE

TOTAL FOR ALL FILES

L79 50 L72 AND (X-RAY OR THREE DIMENSION STRUCTURE OR X-RAY)

=> dup rem l79

PROCESSING COMPLETED FOR L79

L80 29 DUP REM L79 (21 DUPLICATES REMOVED)

=> d ibib abs 1-29

L80 ANSWER 1 OF 29 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: 2000:346629 BIOSIS

DOCUMENT NUMBER: PREV200000346629

TITLE: The human nm23-H4 gene product is a mitochondrial
nucleoside diphosphate kinase.

AUTHOR(S): Milon, Laurence; Meyer, Philippe; Chiadmi, Mohamed; Munier,
Annie; Johansson, Magnus; Karlsson, Anna; Lascu, Ioan;
Capeau, Jacqueline; Janin, Joel; Lacombe, Marie-Lise
[Reprint author]

CORPORATE SOURCE: Faculte de Medecine Saint-Antoine, INSERM U402, 27 Rue
Chaligny, 75012, Paris, France

SOURCE: Journal of Biological Chemistry, (May 12, 2000) Vol. 275,
No. 19, pp. 14264-14272. print.
CODEN: JBCHA3. ISSN: 0021-9258.

DOCUMENT TYPE: Article

LANGUAGE: English

ENTRY DATE: Entered STN: 16 Aug 2000

Last Updated on STN: 7 Jan 2002

AB We demonstrate here the catalytic activity and subcellular localization of the Nm23-H4 protein, product of nm23-H4, a new member of the human nm23/**nucleoside diphosphate (NDP) kinase** gene family (Milon, L., Rousseau-Merck, M., Munier, A., Erent, M., Lascu, I., Capeau, J., and Lacombe, M. L. (1997) Hum. Genet. 99, 550-557). Nm3-H4 was synthesized in escherichia coli as the full-length protein and as a truncated form missing the N-terminal extension characteristic of mitochondrial targeting. The truncated form possesses NDP **kinase** activity, whereas the full-length protein is inactive, suggesting that the extension prevents enzyme folding and/or activity. **X-ray** crystallographic analysis was performed on active truncated Nm23-H4. Like other eukaryotic NDP **kinases**, it is a hexamer. Nm23-H4 naturally possesses a serine residue at position 129, equivalent to the K-pn mutation of the Drosophila NDP **kinase**. The **x-ray** structure shows that the presence of Ser129 has local structural effects that weaken subunit interactions. Site-directed mutagenesis shows that the serine is responsible for the lability of Nm23-H4 to heat and urea treatment, because the S129P mutant is greatly stabilized. Examination of human embryonic kidney 293 cells transfected with green fluorescent protein fusions by confocal microscopy shows a specific mitochondrial localization of Nm23-H4 that was also demonstrated by Western blot analysis of subcellular fractions of these cells. Import into mitochondria is accompanied by cleavage of the N-terminal extension that results in NDP **kinase** activity. Submitochondrial fractionation indicates that Nm23-H4 is associated with mitochondrial membranes, possibly to the contact sites between the outer and inner membranes.

L80 ANSWER 2 OF 29 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: 2001:49122 BIOSIS

DOCUMENT NUMBER: PREV200100049122
TITLE: **Nucleoside** diphosphate **kinase** from the hyperthermophilic archaeon *Methanococcus jannaschii*: Overexpression, crystallization and preliminary X-ray crystallographic analysis.
AUTHOR(S): Min, Kyeongsik; Song, Hyun Kyu; Chang, Changsoo; Lee, Jae Young; Eom, Soo Hyun; Kim, Kyeong Kyu; Yu, Yeon Gyu; Suh, Se Won [Reprint author]
CORPORATE SOURCE: Department of Chemistry, College of Natural Sciences, Seoul National University, Seoul, 151-742, South Korea
sewonsuh@snu.ac.kr
SOURCE: Acta Crystallographica Section D Biological Crystallography, (November, 2000) Vol. 56, No. 11, pp. 1485-1487. print.
ISSN: 0907-4449.
DOCUMENT TYPE: Article
LANGUAGE: English
ENTRY DATE: Entered STN: 24 Jan 2001
Last Updated on STN: 12 Feb 2002

AB **Nucleoside** diphosphate (NDP) **kinase** is a key enzyme in maintaining cellular pools of all **nucleoside** triphosphates. NDP **kinase** from the hyperthermophilic archaeobacterium *Methanococcus jannaschii* has been overexpressed in *Escherichia coli* and crystallized at 297 K using polyethylene glycol 4000 as precipitant. The crystal is hexagonal, belonging to the space group P63, with unit-cell parameters $a = b = 72.89$, $c = 100.87$ Å. The asymmetric unit contains two subunits of NDP **kinase**, with a corresponding crystal volume per protein mass (VM) of 2.38 Å³ Da⁻¹ and a solvent content of 48.3%. Native X-ray diffraction data to 2.30 Å resolution have been collected using synchrotron X-rays.

L80 ANSWER 3 OF 29 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: 2000:241228 BIOSIS
DOCUMENT NUMBER: PREV200000241228
TITLE: Crystal structure of adenosine **kinase** from *Toxoplasma gondii* at 1.8 Å resolution.
AUTHOR(S): Cook, William J.; DeLucas, Lawrence J.; Chattopadhyay, Debasish [Reprint author]
CORPORATE SOURCE: Center for Macromolecular Crystallography, University of Alabama at Birmingham, Birmingham, AL, 35294, USA
SOURCE: Protein Science, (April, 2000) Vol. 9, No. 4, pp. 704-712. print.
ISSN: 0961-8368.
DOCUMENT TYPE: Article
LANGUAGE: English
ENTRY DATE: Entered STN: 14 Jun 2000
Last Updated on STN: 5 Jan 2002

AB Human infection with *Toxoplasma gondii* is an important cause of morbidity and mortality. Protozoan parasites such as *T. gondii* are incapable of de novo purine biosynthesis and must acquire purines from their host, so the purine salvage pathway offers a number of potential targets for antiparasitic chemotherapy. In *T. gondii* tachyzoites, adenosine is the predominantly salvaged purine **nucleoside**, and thus adenosine **kinase** is a key enzyme in the purine salvage pathway of this parasite. The structure of *T. gondii* adenosine **kinase** was solved using molecular replacement and refined by simulated annealing at 1.8 Å resolution to an R-factor of 0.214. The overall structure and the active site geometry are similar to human adenosine **kinase**, although there are significant differences. The *T. gondii* adenosine **kinase** has several unique features compared to the human sequence, including a five-residue deletion in one of the four linking segments between the two domains, which is probably responsible for a major change in the orientation of the two domains with respect to each other. These structural differences suggest the possibility of developing specific inhibitors of the parasitic enzyme.

L80 ANSWER 4 OF 29 EMBASE COPYRIGHT 2004 ELSEVIER INC. ALL RIGHTS RESERVED. on STN

ACCESSION NUMBER: 2000342324 EMBASE
TITLE: The human Nm23/**Nucleoside** diphosphate **kinases**.

AUTHOR: Lacombe M.-L.; Milon L.; Munier A.; Mehus J.G.; Lambeth D.O.
 CORPORATE SOURCE: M.-L. Lacombe, INSERM U402, Faculte de Medecine Saint-Antoine, 75012 Paris, France
 SOURCE: Journal of Bioenergetics and Biomembranes, (2000) 32/3 (247-258).
 Refs: 96
 ISSN: 0145-479X CODEN: JBBID4
 COUNTRY: United States
 DOCUMENT TYPE: Journal; General Review
 FILE SEGMENT: 029 Clinical Biochemistry
 LANGUAGE: English
 SUMMARY LANGUAGE: English

AB Biochemical experiments over the past 40 years have shown that **nucleoside** diphosphate (NDP) **kinase** activity, which catalyzes phosphoryl transfer from a **nucleoside** triphosphate to a **nucleoside** diphosphate, is ubiquitously found in organisms from **bacteria** to human. Over the past 10 years, eight human genes of the nm23/NDP **kinase** family have been discovered that can be separated into two groups based on analysis of their sequences. In addition to catalysis, which may not be exhibited by all isoforms, evidence for regulatory roles has come recently from the discovery of the genes nm23 and awd, which encode NDP **kinases** and are involved in tumor metastasis and Drosophila development, respectively. Current work shows that the human NDP **kinase** genes are differentially expressed in tissues and that their products are targeted to different subcellular locations. This suggests that Nm23/NDP **kinases** possess different, but specific, functions within the cell, depending on their localization. The roles of NDP **kinases** in metabolic pathways and nucleic acid synthesis are discussed.

L80 ANSWER 5 OF 29 MEDLINE on STN DUPLICATE 1

ACCESSION NUMBER: 2002042201 MEDLINE
 DOCUMENT NUMBER: PubMed ID: 11768306
 TITLE: Quaternary structure of **nucleoside** diphosphate **kinases**.

AUTHOR: Lascu L; Giartosio A; Ransac S; Erent M
 CORPORATE SOURCE: Institut de Biochimie et Genetique Cellulaires, UMR 5095 University of Bordeaux-2 and CNRS, France..
 ioan.lascu@ibgc.u-bordeaux2.fr
 SOURCE: Journal of bioenergetics and biomembranes, (2000 Jun) 32 (3) 227-36. Ref: 81
 Journal code: 7701859. ISSN: 0145-479X.
 PUB. COUNTRY: United States
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 General Review; (REVIEW)
 (REVIEW, TUTORIAL)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals
 ENTRY MONTH: 200207
 ENTRY DATE: Entered STN: 20020124
 Last Updated on STN: 20020713
 Entered Medline: 20020712

AB **Nucleoside** (NDP) diphosphate **kinases** are oligomeric enzymes. Most are hexameric, but some **bacterial** enzymes are tetrameric. Hexamers and tetramers are constructed by assembling identical dimers. The hexameric structure is important for protein stability, as demonstrated by studies with natural mutants (the Killer-of-prune mutant of Drosophila NDP **kinase** and the S120G mutant of the human NDP **kinase** A in neuroblastomas) and with mutants obtained by site-directed mutagenesis. It is also essential for enzymic activity. The function of the tetrameric structure is unclear.

L80 ANSWER 6 OF 29 MEDLINE on STN

ACCESSION NUMBER: 2000133169 MEDLINE
 DOCUMENT NUMBER: PubMed ID: 10666613
 TITLE: Crystallization and preliminary X-ray analysis of the thymidylate **kinase** from Mycobacterium tuberculosis.

AUTHOR: Li de la Sierra I; Munier-Lehmann H; Gilles A M; Barzu O; Delarue M

CORPORATE SOURCE: Unite de Biochimie Structurale, Institut Pasteur, 28 Rue du
Dr Roux, 75724, Paris CEDEX 15, France.

SOURCE: Acta crystallographica. Section D, Biological
crystallography, (2000 Feb) 56 (Pt 2) 226-8.
Journal code: 9305878. ISSN: 0907-4449.

PUB. COUNTRY: Denmark

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

FILE SEGMENT: Priority Journals

ENTRY MONTH: 200004

ENTRY DATE: Entered STN: 20000413
Last Updated on STN: 20000413
Entered Medline: 20000405

AB Mycobacterium tuberculosis thymidylate **kinase** complexed with the
substrate deoxythymidine monophosphate was crystallized in the hexagonal
space group P6(5)22 or P6(1)22, with unit-cell parameters a = b = 76.62, c
= 134.38 A and one single monomer of 23 kDa in the asymmetric unit.
Cryo-cooled crystals diffract at 1.94 A resolution using synchrotron
radiation.

L80 ANSWER 7 OF 29 MEDLINE on STN DUPLICATE 2

ACCESSION NUMBER: 2002042200 MEDLINE

DOCUMENT NUMBER: PubMed ID: 11768305

TITLE: Three-dimensional structure of **nucleoside**
diphosphate **kinase**.

AUTHOR: Janin J; Dumas C; Morera S; Xu Y; Meyer P; Chiadmi M;
Cherfils J

CORPORATE SOURCE: Laboratoire d'Enzymologie et de Biochimie Structurales CNRS
UPR9063, Gif-sur-Yvette, France.. janin@lebs.cnrs-gif.fr

SOURCE: Journal of bioenergetics and biomembranes, (2000 Jun) 32
(3) 215-25. Ref: 46
Journal code: 7701859. ISSN: 0145-479X.

PUB. COUNTRY: United States

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
General Review; (REVIEW)
(REVIEW, TUTORIAL)

LANGUAGE: English

FILE SEGMENT: Priority Journals

ENTRY MONTH: 200207

ENTRY DATE: Entered STN: 20020124
Last Updated on STN: 20020713
Entered Medline: 20020712

AB Three-dimensional structures are known from **X-ray**
studies of the **nucleoside** diphosphate (NDP) **kinase** of
many organisms from **bacteria** to human. All NDP **kinases**
have subunits of about 150 residues with a very similar fold based on the
alphabeta sandwich or ferredoxin fold. This fold is found in many
nucleotide or polynucleotide-binding proteins with no sequence
relationship to NDP **kinase**. This common fold is augmented here
with specific features: a surface alpha-helix hairpin, the Kpn loop, and
the C-terminal extension. The alpha-helix hairpin and Kpn loop make up
the nucleotide binding site, which is unique to NDP **kinase** and
different from that of other **kinases** or ATPases. The Kpn loop
and the C-terminal extension are also involved in the quaternary
structure. Whereas all known eukaryotic NDP **kinases**, including
mitochondrial enzymes, are hexamers, some **bacterial** enzymes are
tetramers. However, hexameric and tetrameric NDP **kinases** are
built from the same dimer. The structural environment of the active
histidine is identical in all. The nucleotide binding site is also fully
conserved, except for a feature implicating C-terminal residues in the
hexamer, but not in the tetramer. Structural data on the native and
phosphorylated enzyme, complexes with substrates, inhibitor, and a
transition state analog, give a solid basis to a mechanism of phosphate
transfer in which the largest contributors to catalysis are the 3'-OH of
the sugar and the bound Mg2+ in the nucleotide substrate. In contrast, we
still lack structural data relating to DNA binding and other functions of
NDP **kinases**.

L80 ANSWER 8 OF 29 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: 1999:255947 BIOSIS

DOCUMENT NUMBER: PREV199900255947

TITLE: Nucleophilic activation by positioning in phosphoryl transfer catalyzed by **nucleoside diphosphate kinase**.

AUTHOR(S): Admiraal, Suzanne J.; Schneider, Benoit; Meyer, Philippe; Janin, Joel; Veron, Michel; Deville-Bonne, Dominique; Herschlag, Daniel [Reprint author]

CORPORATE SOURCE: Department of Biochemistry, Beckman Center B400, Stanford University, Stanford, CA, 94305-5307, USA

SOURCE: Biochemistry, (April 13, 1999) Vol. 38, No. 15, pp. 4701-4711. print.
CODEN: BICHAW. ISSN: 0006-2960.

DOCUMENT TYPE: Article

LANGUAGE: English

ENTRY DATE: Entered STN: 2 Jul 1999
Last Updated on STN: 2 Jul 1999

AB The nonenzymatic reaction of ATP with a nucleophile to generate ADP and a phosphorylated product proceeds via a dissociative transition state with little bond formation to the nucleophile. Consideration of the dissociative nature of the nonenzymatic transition state leads to the following question: To what extent can the nucleophile be activated in enzymatic phosphoryl transfer? We have addressed this question for the NDP **kinase** reaction. A mutant form of the enzyme lacking the nucleophilic histidine (H122G) can be chemically rescued for ATP attack by imidazole or other exogenous small nucleophiles. The ATP reaction is 50-fold faster with the wild-type enzyme, which has an imidazole nucleophile positioned for reaction by a covalent bond, than with H122G, which employs a noncovalently bound imidazole nucleophile ((kcat/KM)ATP). Further, a 4-fold advantage for imidazole positioned in the nucleophile binding pocket created by the mutation is suggested from comparison of the reaction of H122G and ATP with an imidazole versus a water nucleophile, after correction for the intrinsic reactivities of imidazole and water toward ATP in solution. **X-ray** structural analysis shows no detectable rearrangement of the residues surrounding His 122 upon mutation to Gly 122. The overall rate effect of approx102-fold for the covalent imidazole nucleophile relative to water is therefore attributed to positioning of the nucleophile with respect to the reactive phosphoryl group. This is underscored by the more deleterious effect of replacing ATP with ATPgammaS in the wild-type reaction than in the imidazole-rescued mutant reaction, as follows. For the wild-type, ATPgammaS presumably disrupts positioning between nucleophile and substrate, resulting in a large thio effect of 300-fold, whereas precise alignment is already disrupted in the mutant because there is no covalent bond to the nucleophile, resulting in a smaller thio effect of 10-fold. In summary, the results suggest a catalytic role for activation of the nucleophile by positioning in phosphoryl transfer catalyzed by NDP **kinase**.

L80 ANSWER 9 OF 29 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: 1999:317523 BIOSIS

DOCUMENT NUMBER: PREV199900317523

TITLE: The three-dimensional structures of two isoforms of **nucleoside diphosphate kinase** from bovine retina.

AUTHOR(S): Ladner, Jane E.; Abdulaev, Najmoutin G.; Kakuev, Dmitri L.; Tordova, Maria; Ridge, Kevin D.; Gilliland, Gary L. [Reprint author]

CORPORATE SOURCE: Center for Advanced Research in Biotechnology, National Institute of Standards and Technology and University of Maryland Biotechnology Institute, 9600 Gudelsky Drive, Rockville, MD, 20850, USA

SOURCE: Acta Crystallographica Section D Biological Crystallography, (June, 1999) Vol. 55, No. 6, pp. 1127-1135. print.
ISSN: 0907-4449.

DOCUMENT TYPE: Article

LANGUAGE: English

ENTRY DATE: Entered STN: 17 Aug 1999
Last Updated on STN: 17 Aug 1999

AB The crystal structures of two isoforms of **nucleoside diphosphate kinase** from bovine retina overexpressed in Escherischia coli have been determined to 2.4 ANG resolution. Both the isoforms, NBR-A and NBR-B, are hexameric and the fold of the monomer is in agreement with NDP-

kinase structures from other biological sources. Although the polypeptide chains of the two isoforms differ by only two residues, they crystallize in different space groups. NBR-A crystallizes in space group P212121 with an entire hexamer in the asymmetric unit, while NBR-B crystallizes in space group P43212 with a trimer in the asymmetric unit. The highly conserved nucleotide-binding site observed in other **nucleoside** diphosphate **kinase** structures is also observed here. Both NBR-A and NBR-B were crystallized in the presence of cGMP. The nucleotide is bound with the base in the anti conformation. The NBR-A active site contained both cGMP and GDP each bound at half occupancy. Presumably, NBR-A had retained GDP(or GTP) from the purification process. The NBR-B active site contained only cGMP.

L80 ANSWER 10 OF 29 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
 ACCESSION NUMBER: 1999:415650 BIOSIS
 DOCUMENT NUMBER: PREV199900415650
 TITLE: 2.0 ANG **X-ray** structure of the ternary complex of 7,8-dihydro-6-hydroxymethylpterinpyrophosphokinase from *Escherichia coli* with ATP and a substrate analogue.
 AUTHOR(S): Stammers, David K.; Achari, Aniruddha; Somers, Donald O'N. [Reprint author]; Bryant, Patrick K.; Rosemond, Jane; Scott, David L.; Champness, John N.
 CORPORATE SOURCE: Medicines Research Centre, Glaxo Wellcome R and D, Gunnell's Wood Road, Stevenage, SG1 2NY, UK
 SOURCE: FEBS Letters, (July 30, 1999) Vol. 465, No. 1, pp. 49-53. print.
 CODEN: FEBLAL. ISSN: 0014-5793.
 DOCUMENT TYPE: Article
 LANGUAGE: English
 ENTRY DATE: Entered STN: 18 Oct 1999
 Last Updated on STN: 18 Oct 1999

AB The **X-ray** crystal structure of 7,8-dihydro-6-hydroxymethylpterinpyrophosphokinase (PPPK) in a ternary complex with ATP and a pterin analogue has been solved to 2.0 ANG resolution, giving, for the first time, detailed information of the PPPK/ATP intermolecular interactions and the accompanying conformational change. The first 100 residues of the 158 residue peptide contain a betaalphanbetabetaalphanbetamotif present in several other proteins including **nucleoside** diphosphate **kinase**. Comparative sequence examination of a wide range of prokaryotic and lower eukaryotic species confirms the conservation of the PPPK active site, indicating the value of this *de novo* folate biosynthesis pathway enzyme as a potential target for the development of novel broad-spectrum anti-infective agents.

L80 ANSWER 11 OF 29 MEDLINE on STN
 ACCESSION NUMBER: 1999045634 MEDLINE
 DOCUMENT NUMBER: PubMed ID: 9826650
 TITLE: Structural basis for efficient phosphorylation of 3'-azidothymidine monophosphate by *Escherichia coli* thymidylate **kinase**.
 AUTHOR: Lavie A; Ostermann N; Brundiers R; Goody R S; Reinstein J; Konrad M; Schlichting I
 CORPORATE SOURCE: Department of Physical Biochemistry, Max Planck Institute for Molecular Physiology, Rheinlanddamm 201, 44139 Dortmund, Germany.
 SOURCE: Proceedings of the National Academy of Sciences of the United States of America, (1998 Nov 24) 95 (24) 14045-50. Journal code: 7505876. ISSN: 0027-8424.
 PUB. COUNTRY: United States
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals; AIDS
 OTHER SOURCE: PDB-4TMK; PDB-5TMP
 ENTRY MONTH: 199812
 ENTRY DATE: Entered STN: 19990115
 Last Updated on STN: 19990115
 Entered Medline: 19981228

AB The crystal structures of *Escherichia coli* thymidylate **kinase** (TmkK) in complex with P1-(5'-adenosyl)-P5-(5'-thymidyl)pentaphosphate and P1-(5'-adenosyl)P5-[5'-(3'-azido-3'-deoxythymidine)] pentaphosphate have been solved to 2.0-A and 2.2-A resolution, respectively. The overall

structure of the **bacterial** TmpK is very similar to that of yeast TmpK. In contrast to the human and yeast TmpKs, which phosphorylate 3'-azido-3'-deoxythymidine 5'-monophosphate (AZT-MP) at a 200-fold reduced turnover number (kcat) in comparison to the physiological substrate dTMP, reduction of kcat is only 2-fold for the **bacterial** enzyme. The different kinetic properties toward AZT-MP between the eukaryotic TmpKs and E. coli TmpK can be rationalized by the different ways in which these enzymes stabilize the presumed transition state and the different manner in which a carboxylic acid side chain in the P loop interacts with the deoxyribose of the monophosphate. Yeast TmpK interacts with the 3'-hydroxyl of dTMP through Asp-14 of the P loop in a bidentate manner: binding of AZT-MP results in a shift of the P loop to accommodate the larger substituent. In E. coli TmpK, the corresponding residue is Glu-12, and it interacts in a side-on fashion with the 3'-hydroxyl of dTMP. This different mode of interaction between the P loop carboxylic acid with the 3' substituent of the monophosphate deoxyribose allows the accommodation of an azido group in the case of the E. coli enzyme without significant P loop movement. In addition, although the yeast enzyme uses Arg-15 (a glycine in E. coli) to stabilize the transition state, E. coli seems to use Arg-153 from a region termed Lid instead. Thus, the binding of AZT-MP to the yeast TmpK results in the shift of a catalytic residue, which is not the case for the **bacterial kinase**.

L80 ANSWER 12 OF 29 MEDLINE on STN
 ACCESSION NUMBER: 1998004500 MEDLINE
 DOCUMENT NUMBER: PubMed ID: 9342339
 TITLE: Assigning folds to the proteins encoded by the genome of Mycoplasma genitalium.
 AUTHOR: Fischer D; Eisenberg D
 CORPORATE SOURCE: University of California, Los Angeles-Department of Energy Laboratory of Structural Biology and Molecular Medicine, Molecular Biology Institute, University of California, Los Angeles, Box 951570, Los Angeles, CA 90095-1570, USA.
 SOURCE: Proceedings of the National Academy of Sciences of the United States of America, (1997 Oct 28) 94 (22) 11929-34. Journal code: 7505876. ISSN: 0027-8424.
 PUB. COUNTRY: United States
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals
 ENTRY MONTH: 199712
 ENTRY DATE: Entered STN: 19980109
 Last Updated on STN: 19980109
 Entered Medline: 19971204

AB A crucial step in exploiting the information inherent in genome sequences is to assign to each protein sequence its three-dimensional fold and biological function. Here we describe fold assignment for the proteins encoded by the small genome of Mycoplasma genitalium. The assignment was carried out by our computer server (<http://www.doe-mbi.ucla.edu/people/frsvr/frsvr.html>), which assigns folds to amino acid sequences by comparing sequence-derived predictions with known structures. Of the total of 468 protein ORFs, 103 (22%) can be assigned a known protein fold with high confidence, as cross-validated with tests on known structures. Of these sequences, 75 (16%) show enough sequence similarity to proteins of known structure that they can also be detected by traditional sequence-sequence comparison methods. That is, the difference of 28 sequences (6%) are assignable by the sequence-structure method of the server but not by current sequence-sequence methods. Of the remaining 78% of sequences in the genome, 18% belong to membrane proteins and the remaining 60% cannot be assigned either because these sequences correspond to no presently known fold or because of insensitivity of the method. At the current rate of determination of new folds by **x-ray** and NMR methods, extrapolation suggests that folds will be assigned to most soluble proteins in the next decade.

L80 ANSWER 13 OF 29 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
 ACCESSION NUMBER: 1996:438453 BIOSIS
 DOCUMENT NUMBER: PREV199699152059
 TITLE: **Nucleoside** diphosphate **kinase**: Investigation of the intersubunit contacts by site-directed mutagenesis and crystallography.

AUTHOR(S): Karlsson, Anna; Mesnildrey, Sebastien; Xu, Yingwu; Morera, Solange; Janin, Joel; Veron, Michel [Reprint author]
 CORPORATE SOURCE: Unite de Regulation Enzymatique des Activites Cellulaires, Inst. Pasteur, 25 rue du Dr. Roux, 75724, Paris Cedex 15, France
 SOURCE: Journal of Biological Chemistry, (1996) Vol. 271, No. 33, pp. 19928-19934.
 CODEN: JBCHA3. ISSN: 0021-9258.
 DOCUMENT TYPE: Article
 LANGUAGE: English
 ENTRY DATE: Entered STN: 26 Sep 1996
 Last Updated on STN: 26 Sep 1996

AB NDP **kinase** from Dictyostelium was mutated by site-directed mutagenesis at positions indicated by structural data to be involved in the trimer interface. The mutants were substitutions at residue Pro-100 (P100S and P100G) and deletions of 1-5 residues at the C terminus. Single mutants yielded proteins that kept both activity and hexameric structure. However, they were severely affected in their stability toward temperature and urea denaturation. When the P100S mutation was combined with any of the C-terminal deletions, the enzyme lost most of its activity and dissociated into dimers. Crystallographic analysis of the P100S protein was performed at 2.6 Å resolution. The **x-ray** structure showed no direct alteration of intersubunits contacts at residue 100, but an induced disruption of the interaction between Asp-115 and the C terminus of another subunit. The substitution of proline 100 to serine corresponds to the Killer-of-prune mutation in Drosophila. Consequences of the mutation are discussed in view of the structural and biochemical properties observed in the mutant Dictyostelium protein.

L80 ANSWER 14 OF 29 MEDLINE on STN DUPLICATE 3
 ACCESSION NUMBER: 96279323 MEDLINE
 DOCUMENT NUMBER: PubMed ID: 8663370
 TITLE: Thermal stability of hexameric and tetrameric **nucleoside** diphosphate **kinases**. Effect of subunit interaction.
 AUTHOR: Giartosio A; Erent M; Cervoni L; Morera S; Janin J; Konrad M; Lascu I
 CORPORATE SOURCE: Dipartimento di Scienze Biochimiche "A. Rossi Fanelli" and Center of Molecular Biology of C.N.R., Universita degli Studi "La Sapienza, " 00185 Roma, Italy.
 SOURCE: Journal of biological chemistry, (1996 Jul 26) 271 (30) 17845-51.
 Journal code: 2985121R. ISSN: 0021-9258.
 PUB. COUNTRY: United States
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals
 OTHER SOURCE: PDB-INCL
 ENTRY MONTH: 199609
 ENTRY DATE: Entered STN: 19960912
 Last Updated on STN: 19970203
 Entered Medline: 19960903

AB The eukaryotic **nucleoside** diphosphate (NDP) **kinases** are hexamers, while the **bacterial** NDP **kinases** are tetramers made of small, single domain subunits. These enzymes represent an ideal model for studying the effect of subunit interaction on protein stability. The thermostability of NDP **kinases** of each class was studied by differential scanning calorimetry and biochemical methods. The hexameric NDP **kinase** from Dictyostelium discoideum displays one single, irreversible differential scanning calorimetry peak (T_m 62 degrees C) over a broad protein concentration, indicating a single step denaturation. The thermal stability of the protein was increased by ADP. The P105G substitution, which affects a loop implicated in subunit contacts, yields a protein that reversibly dissociates to folded monomers at 38 degrees C before the irreversible denaturation occurs (T_m 47 degrees C). ADP delays the dissociation, but does not change the T_m. These data indicate a "coupling" of the quaternary structure with the tertiary structure in the wild-type, but not in the mutated protein. We describe the **x-ray** structure of the P105G mutant at 2.2-Å resolution. It is very similar to that of the wild-type protein. Therefore, a minimal change in the structure leads to a dramatic change of

protein thermostability. The NDP **kinase** from *Escherichia coli* behaves like the P105G mutant of the *Dictyostelium* NDP **kinase**. The detailed study of their thermostability is important, since biological effects of thermolabile NDP **kinases** have been described in several organisms.

L80 ANSWER 15 OF 29 MEDLINE on STN DUPLICATE 4
 ACCESSION NUMBER: 96162036 MEDLINE
 DOCUMENT NUMBER: PubMed ID: 8576266
 TITLE: CMP **kinase** from *Escherichia coli* is structurally related to other **nucleoside** monophosphate **kinases**.
 AUTHOR: Bucurenci N; Sakamoto H; Briozzo P; Palibroda N; Serina L; Sarfati R S; Labesse G; Briand G; Danchin A; Barzu O; Gilles A M
 CORPORATE SOURCE: Unite de Biochimie des Regulations Cellulaires, Institut Pasteur, Paris, France.
 SOURCE: Journal of biological chemistry, (1996 Feb 2) 271 (5) 2856-62.
 Journal code: 2985121R. ISSN: 0021-9258.
 PUB. COUNTRY: United States
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals
 ENTRY MONTH: 199603
 ENTRY DATE: Entered STN: 19960321
 Last Updated on STN: 19960321
 Entered Medline: 19960312

AB CMP **kinase** from *Escherichia coli* is a monomeric protein of 225 amino acid residues. The protein exhibits little overall sequence similarities with other known NMP **kinases**. However, residues involved in binding of substrates and/or in catalysis were found conserved, and sequence comparison suggested conservation of the global fold found in adenylate **kinases** or in several CMP/UMP **kinases**. The enzyme was purified to homogeneity, crystallized, and analyzed for its structural and catalytic properties. The crystals belong to the hexagonal space group P6(3), have unit cell parameters $a = b = 82.3$ A and $c = 60.7$ A, and diffract **x-rays** to a 1.9 A resolution. The **bacterial** enzyme exhibits a fluorescence emission spectrum with maximum at 328 nm upon excitation at 295 nm, which suggests that the single tryptophan residue (Trp30) is located in a hydrophobic environment. Substrate specificity studies showed that CMP **kinase** from *E. coli* is active with ATP, dATP, or GTP as donors and with CMP, dCMP, and arabinofuranosyl-CMP as acceptors. This is in contrast with CMP/UMP **kinase** from *Dictyostelium discoideum*, an enzyme active on CMP or UMP but much less active on the corresponding deoxynucleotides. Binding of CMP enhanced the affinity of *E. coli* CMP **kinase** for ATP or ADP, a particularity never described in this family of proteins that might explain inhibition of enzyme activity by excess of **nucleoside** monophosphate.

L80 ANSWER 16 OF 29 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
 ACCESSION NUMBER: 1995:367921 BIOSIS
 DOCUMENT NUMBER: PREV199598382221
 TITLE: The 1.9 A crystal structure of a **nucleoside** diphosphate **kinase** complex with adenosine 3',5'-cyclic monophosphate: Evidence for competitive inhibition.
 AUTHOR(S): Strelkov, Sergei V.; Perisic, Olga; Webb, Philip A.; Williams, Roger L. [Reprint author]
 CORPORATE SOURCE: Cent. Protein Eng., Med. Res. Council, Centre Hills Rd., Cambridge CB2 2QH, UK
 SOURCE: Journal of Molecular Biology, (1995) Vol. 249, No. 3, pp. 665-674.
 CODEN: JMOBAK. ISSN: 0022-2836.
 DOCUMENT TYPE: Article
 LANGUAGE: English
 ENTRY DATE: Entered STN: 30 Aug 1995
 Last Updated on STN: 10 Oct 1995

AB The **X-ray** structure of *Myxococcus xanthus* **nucleoside** diphosphate (NDP) **kinase** complexed with

adenosine 3',5'-cyclic monophosphate (cAMP) has been determined. The structure was solved by difference Fourier analysis. The refined structure has a crystallographic R-factor of 0.17 at 1.9 Å resolution. The phosphoryl group and ribose moiety make extensive polar interactions with the protein, whereas the base interacts only with two hydrophobic residues. The comparison with the structure of the enzyme complex with the substrate adenosine diphosphate (ADP) reported earlier shows that cAMP and ADP interact similarly with the enzyme. The base of the cAMP is present in two conformations, syn and anti, with respect to the sugar. The syn conformer is dominant. Based on the effect of cAMP on phosphorylation of the human NDP **kinase** NM23, it had been proposed that cAMP might interact with NDP **kinase** in a manner distinct from other nucleotides. However, the structure of the *M. xanthus* NDP **kinase**/cAMP complex indicates that the nucleotide is a competitive inhibitor of the enzyme and occupies the usual nucleotide site. Kinetic assays of the NDP **kinase** activity in the presence of cAMP were done. Their results are consistent with a competitive character of the cAMP inhibition.

L80 ANSWER 17 OF 29 MEDLINE on STN
 ACCESSION NUMBER: 95393019 MEDLINE
 DOCUMENT NUMBER: PubMed ID: 7663945
 TITLE: Movie of the structural changes during a catalytic cycle of **nucleoside** monophosphate **kinases**.
 AUTHOR: Vornheim C; Schlauderer G J; Schulz G E
 CORPORATE SOURCE: Institut für Organische Chemie und Biochemie, Albert-Ludwigs-Universität, Freiburg im Breisgau, Germany.
 SOURCE: Structure (London, England), (1995 May 15) 3 (5) 483-90. Journal code: 9418985. ISSN: 0969-2126.
 PUB. COUNTRY: ENGLAND: United Kingdom
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals
 ENTRY MONTH: 199510
 ENTRY DATE: Entered STN: 19951020
 Last Updated on STN: 19951020
 Entered Medline: 19951012

AB BACKGROUND: There are 17 crystal structures of **nucleoside** monophosphate **kinases** known. As expected for **kinases**, they show large conformational changes upon binding of substrates. These are concentrated in two chain segments, or domains, of 30 and 38 residues that are involved in binding of the substrates N1TP and N2MP (**nucleoside** tri- and monophosphates with bases N1 and N2), respectively. RESULTS: After aligning the 17 structures on the main parts of their polypeptide chains, two domains in various conformational states were revealed. These states were caused by bound substrate (or analogues) and by crystal-packing forces, and ranged between a 'closed' conformation and a less well defined 'open' conformation. The structures were visually sorted yielding an approximately evenly spaced series of domain states that outlines the closing motions when the substrates bind. The packing forces in the crystals are weak, leaving the natural domain trajectories essentially intact. Packing is necessary, however, to produce stable intermediates. The ordered experimental structures were then recorded as still pictures of a movie and animated to represent the motions of the molecule during a catalytic cycle. The motions were smoothed out by adding interpolated structures to the observed ones. The resulting movies are available through the World Wide Web (http://bio5.chemie.uni-freiburg.de/ak_movie.html). CONCLUSIONS: Given the proliferating number of homologous proteins known to exist in different conformational states, it is becoming possible to outline the motions of chain segments and combine them into a movie, which can then represent protein action much more effectively than static pictures alone are able to do.

L80 ANSWER 18 OF 29 MEDLINE on STN DUPLICATE 5
 ACCESSION NUMBER: 95055729 MEDLINE
 DOCUMENT NUMBER: PubMed ID: 7966307
 TITLE: Refined **X-ray** structure of *Dictyostelium discoideum* **nucleoside** diphosphate **kinase** at 1.8 Å resolution.
 AUTHOR: Morera S; LeBras G; Lascu I; Lacombe M L; Veron M; Janin J
 CORPORATE SOURCE: Laboratoire de Biologie Structurale, UMR 9920

SOURCE: CNRS-Universite Paris-Sud, Gif-sur-Yvette, France.
 Journal of molecular biology, (1994 Nov 11) 243 (5) 873-90.
 Journal code: 2985088R. ISSN: 0022-2836.
 PUB. COUNTRY: ENGLAND: United Kingdom
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals
 ENTRY MONTH: 199412
 ENTRY DATE: Entered STN: 19950110
 Last Updated on STN: 19950110
 Entered Medline: 19941213

AB The **X-ray** structure of the **nucleoside**
 diphosphate **kinase** (NDP **kinase**) from Dictyostelium
 discoideum has been refined at 1.8 A resolution from a hexagonal crystal
 form with a 17 kDa monomer in its asymmetric unit. The atomic model was
 derived from the previously determined structure of a point mutant of the
 protein. It contains 150 amino acid residues out of 155, and 95 solvent
 molecules. The R-factor is 0.196 and the estimated accuracy of the
 average atomic position, 0.25 A. The Dictyostelium structure is described
 in detail and compared to those of Drosophila and Myxococcus xanthus NDP
kinases. The protein is a hexamer with D3 symmetry. Residues 8
 to 138 of each subunit form a globular alpha/beta domain. The
 four-stranded beta-sheet is antiparallel; its topology is different from
 other phosphate transfer enzymes, and also from the HPr protein which,
 like NDP **kinase**, carries a phosphorylated histidine. The same
 topology is nevertheless found in several other proteins that bind
 mononucleotides, RNA or DNA. Strand connections in NDP **kinase**
 involve alpha-helices and a 20-residue segment called the Kpn loop. The
 beta-sheet is regular except for a beta-bulge in edge strand beta 2 and a
 gamma-turn at residue Ile120 just preceding strand beta 4. The latter may
 induce strain in the main chain near the active site His122. The alpha 1
 beta 2 motif participates in forming dimers within the hexamer, helices
 alpha 1 and alpha 3, the Kpn loop and C terminus, in forming trimers. The
 subunit fold and dimer interactions found in Dictyostelium are conserved
 in other NDP **kinases**. Trimer interactions probably occur in all
 eukaryotic enzymes. They are absent in the **bacterial** Myxococcus
 xanthus enzyme which is a tetramer, even though the subunit structure is
 very similar. In Dictyostelium, contacts between Kpn loops near the
 3-fold axis block access to a central cavity lined with polar residues and
 filled with well-defined solvent molecules. Biochemical data on point
 mutants highlight the contribution of the Kpn loop to protein stability.
 In Myxococcus, the Kpn loops are on the tetramer surface and their
 sequence is poorly conserved. Yet, their conformation is maintained and
 they make a similar contribution to the substrate binding site.

L80 ANSWER 19 OF 29 SCISEARCH COPYRIGHT 2004 THOMSON ISI on STN
 ACCESSION NUMBER: 94:47583 SCISEARCH
 THE GENUINE ARTICLE: MR493
 TITLE: ADENOSINE 5'-DIPHOSPHATE BINDING AND THE ACTIVE-SITE OF
NUCLEOSIDE DIPHOSPHATE **KINASE**
 AUTHOR: MORERA S; LASCU I; DUMAS C; LEBRAS G; BRIOZZO P; VERON M;
 JANIN J (Reprint)
 CORPORATE SOURCE: UNIV PARIS SUD, BIOL STRUCT LAB, CNRS, UMR 9920, BAT 34, 1
 AVE TERRASSE, F-91198 GIF SUR YVETTE, FRANCE (Reprint);
 UNIV PARIS SUD, BIOL STRUCT LAB, CNRS, UMR 9920, BAT 34, 1
 AVE TERRASSE, F-91198 GIF SUR YVETTE, FRANCE; INST
 PASTEUR, UNITE BIOCHIM CELLULAIRE, CNRS, URA 1129, F-75724
 PARIS 15, FRANCE
 COUNTRY OF AUTHOR: FRANCE
 SOURCE: BIOCHEMISTRY, (18 JAN 1994) Vol. 33, No. 2, pp. 459-467.
 ISSN: 0006-2960.
 DOCUMENT TYPE: Article; Journal
 FILE SEGMENT: LIFE
 LANGUAGE: ENGLISH
 REFERENCE COUNT: 43

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB The **X-ray** structure of **nucleoside**
 diphosphate **kinase** (NDP **kinase**) from the slime mold
 Dictyostelium discoideum has been determined to 2.2-angstrom resolution
 and refined to an R-factor of 0.19 with and without bound ADP-Mg2+. The
 nucleotide binds near His 122, a residue which becomes phosphorylated

during the catalytic cycle. The mode of binding is different from that observed in other phosphokinases, and it involves no glycine-rich sequence. The adenine base makes only nonpolar contacts with the protein. It points outside, explaining the lack of specificity of NDP **kinase** toward the base. The ribose 2'- and 3'-hydroxyls and the pyrophosphate moiety are H-bonded to polar side chains. A Mg²⁺ ion bridges the alpha- to the beta-phosphate which approaches the imidazole group of His 122 from the Ndelta side. The geometry at the active site in the ADP-Mg²⁺ complex suggests a mechanism for catalysis whereby the gamma-phosphate of a **nucleoside** triphosphate can be transferred onto His 122 with a minimum of atomic motion.

L80 ANSWER 20 OF 29 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: 1994:396526 BIOSIS

DOCUMENT NUMBER: PREV199497409526

TITLE: The closed conformation of a highly flexible protein: The structure of E. coli adenylate **kinase** with bound AMP and AMPPNP.

AUTHOR(S): Berry, Michael B.; Meador, Bill; Bilderback, Tim; Liang, Peng; Glaser, Michael; Phillips, George N., Jr. [Reprint author]

CORPORATE SOURCE: Dep. Biochem. Cell Biol., P.O. Box 1892, Rice Univ., Houston, TX 77251, USA

SOURCE: Proteins Structure Function and Genetics, (1994) Vol. 19, No. 3, pp. 183-198.
CODEN: PSFGEY. ISSN: 0887-3585.

DOCUMENT TYPE: Article

LANGUAGE: English

ENTRY DATE: Entered STN: 14 Sep 1994

Last Updated on STN: 12 Oct 1994

AB The structure of E. coli adenylate **kinase** with bound AMP and AMPPNP at 2.0 Å resolution is presented. The protein crystallizes in space group C2 with two molecules in the asymmetric unit, and has been refined to an R factor of 20.1% and an R-free of 31.6%. In the present structure, the protein is in the closed (globular) form with the large flexible lid domain covering the AMPPNP molecule. Within the protein, AMP and AMPPNP, an ATP analog, occupy the AMP and ATP sites respectively, which had been suggested by the most recent crystal structure of E. coli adenylate **kinase** with Ap-5A bound (Muller and Schulz. 1992, ref. 1) and prior fluorescence studies (Liang et al., 1991, ref. 2). The binding of substrates and the positions of the active site residues are compared between the present structure and the E. coli adenylate **kinase**/Ap-5A structure. We failed to detect a peak in the density map corresponding to the Mg-2+ ion which is required for catalysis, and its absence has been attributed to the use of ammonium sulfate in the crystallization solution. Finally, a comparison is made between the present structure and the structure of the heavy chain of muscle myosin.

L80 ANSWER 21 OF 29 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: 1993:392679 BIOSIS

DOCUMENT NUMBER: PREV199396067979

TITLE: Structure-based design of inhibitors of purine

nucleoside phosphorylase: 2. 9-Alicyclic and 9-heteroalicyclic derivatives of 9-deazaguanine.

AUTHOR(S): Secrist, John A. Iii; Niwas, Shri; Rose, Jerry D.; Babu, Y. Sudhakar; Bugg, Charles E.; Erion, Mark D.; Guida, Wayne C.; Ealick, Steven E.; Montgomery, John A. [Reprint author]

CORPORATE SOURCE: BioCryst Pharmaceuticals Inc., 2190 Parkway Lake Drive, Birmingham, AL 35244, USA

SOURCE: Journal of Medicinal Chemistry, (1993) Vol. 36, No. 13, pp. 1847-1854.

CODEN: JMCMAR. ISSN: 0022-2623.

DOCUMENT TYPE: Article

LANGUAGE: English

ENTRY DATE: Entered STN: 23 Aug 1993

Last Updated on STN: 3 Jan 1995

AB Alicyclic and heteroalicyclic derivatives of 9-deazaguanine (2-amino-1,5-dihydro-4H-pyrrolo(3,2-d)(pyrimidin-4-one)) are, with one exception, potent inhibitors of purine **nucleoside** phosphorylase (PNP) equaling the corresponding 9-arylmethyl derivatives previously investigated. The mode of binding of these compounds to PNP was

determined by **X-ray** crystallography.

L80 ANSWER 22 OF 29 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
ACCESSION NUMBER: 1994:116367 BIOSIS
DOCUMENT NUMBER: PREV199497129367
TITLE: Crystal structure of *Myxococcus xanthus* **nucleoside**
diphosphate **kinase** and its interaction with a
nucleotide substrate at 2.0 Å resolution.
AUTHOR(S): Williams, Roger L. [Reprint author]; Oren, Deena A.;
Munoz-Dorado, Jose; Inouye, Sumiko; Inouye, Masayori;
Arnold, Edward
CORPORATE SOURCE: Center Advanced Biotechnol. Med., Rutgers Univ. Chem. Dep.,
679 Hoes Lane, Piscataway, NJ 08854-5638, USA
SOURCE: Journal of Molecular Biology, (1993) Vol. 234, No. 4, pp.
1230-1247.
CODEN: JMOBAK. ISSN: 0022-2836.
DOCUMENT TYPE: Article
LANGUAGE: English
ENTRY DATE: Entered STN: 14 Mar 1994
Last Updated on STN: 14 Mar 1994

AB The **X-ray** crystallographic structure of
nucleoside diphosphate (NDP) **kinase** from *Myxococcus*
xanthus has been determined using multiple isomorphous replacement
techniques and refined at 2.0 Å resolution to a crystallographic
R-factor of 0.17. This is the first report of the structure of an
enzymatically active NDP **kinase** and of the enzyme with a bound
nucleotide. The structure has been determined in P4-32-12 and I222
crystal forms. The enzyme monomer consists of a four-stranded
antiparallel beta-sheet. The surfaces of the sheet are partially covered
with five helical segments. There are two protein molecules in the
asymmetric unit of the tetragonal crystal form. They form a dimer with an
extensive interface in which 1092 Å² per monomer is buried. The
majority of the contact area in the dimer interface is between hydrophobic
or aromatic residues. Two dimers are related by a crystallographic 2-fold
axis to yield a tetramer. This tetramer is also present in the
orthorhombic crystals; however, in this case, the 222 symmetry is entirely
crystallographic. Upon tetramer formation, an additional 473 Å² of
solvent-accessible surface area from each monomer becomes buried. The
interface between dimers in the tetramer is stabilized by salt bridges.
Equilibrium sedimentation studies are consistent with the enzyme being a
tetramer in solution. The structure of a complex of adenosine diphosphate
(ADP) with the enzyme was determined and reveals that most of the
nucleotide interactions with the protein are with the pyrophosphate and
ribose groups, while the base has no hydrogen bonds with the protein and
interacts only by stacking with the side chain of Phe59. The Mg-2+
interacts with the pyrophosphate of the ADP and via a solvent molecule
with the side chain of the conserved Asp120 residue. The mode of
interaction with the nucleotide is novel, with the nucleotide binding at
the side of the beta-sheet. The structures of the nucleotide in crystals
grown in the presence or absence of Mg-2+ are essentially identical. In
addition, the phosphotransfer reaction from adenosine triphosphate (ATP)
to the enzyme can occur without Mg-2+. This suggests that only the second
step of the reaction in which the enzyme transfers the phosphate to a
nucleoside diphosphate acceptor is significantly catalyzed by the
metal.

L80 ANSWER 23 OF 29 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
ACCESSION NUMBER: 1992:475431 BIOSIS
DOCUMENT NUMBER: PREV199294106806; BA94:106806
TITLE: **X-RAY** STRUCTURE OF **NUCLEOSIDE**
DIPHOSPHATE **KINASE**.
AUTHOR(S): DUMAS C [Reprint author]; LASCU I; MORERA S; GLASER P;
FOURME R; WALLET V; LACOMBE M-L; VERON M; JANIN J
CORPORATE SOURCE: LABORATOIRE BIOLOGIE STRUCTURALE, BAT 433, UMR 9920
CNRS-UNIVERSITE PARIS-SUD, 91405 ORSAY, FR
SOURCE: EMBO (European Molecular Biology Organization) Journal,
(1992) Vol. 11, No. 9, pp. 3203-3208.
CODEN: EMJODG. ISSN: 0261-4189.
DOCUMENT TYPE: Article
FILE SEGMENT: BA
LANGUAGE: ENGLISH

ENTRY DATE: Entered STN: 27 Oct 1992
Last Updated on STN: 28 Oct 1992

AB The **X-ray** structure of a point mutant of **nucleoside diphosphate kinase** (NDP **kinase**) from *Dictyostelium discoideum* has been determined to 2.2 .ANG. resolution. The enzyme is a hexamer made of identical subunits with a novel mononucleotide binding fold. Each subunit contains an .alpha./.beta. domain with a four stranded, antiparallel .beta.-sheet. The topology is different from adenylate **kinase**, but identical to the allosteric domain of *Escherichia coli* ATCase regulatory subunits, which bind mononucleotides at an equivalent position. Dimer contacts between NDP **kinase** subunits within the hexamer are similar to those in ATCase. Trimer contacts involve a large loop of polypeptide chain that bears the site of the Pro .fwdarw. Ser substitution in Killer of prune (K-pm) mutants of the highly homologous *Drosophila* enzyme. Properties of *Drosophila* NDP **kinase**, the product of the *awd* developmental gene, and of the human enzyme, the product of the *nm23* genes in tumorigenesis, are discussed in view of the three-dimensional structure and of possible interactions of NDP **kinase** with other nucleotide binding proteins.

L80 ANSWER 24 OF 29 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
ACCESSION NUMBER: 1991:217941 BIOSIS
DOCUMENT NUMBER: PREV199140103776; BR40:103776
TITLE: STRUCTURE DETERMINATION OF **NUCLEOSIDE DIPHOSPHATE KINASE** FROM *MYXOCOCCUS-XANTHUS* AND MOLECULAR MODELING OF NUCLEOTIDE SOLVATION.
AUTHOR(S): WILLIAMS R L [Reprint author]; MUNOZ-DORADO J; GRANT A G; JACOBO-MOLINA A; INOUE M; INOUE S; ARNOLD E
CORPORATE SOURCE: CENT ADVANCED BIOTECHNOLOGY MEDICINE, PISCATAWAY, NJ, USA
SOURCE: Biophysical Journal, (1991) Vol. 59, No. 2 PART 2, pp. 295A.
Meeting Info.: THIRTY-FIFTH ANNUAL MEETING OF THE BIOPHYSICAL SOCIETY, SAN FRANCISCO, CALIFORNIA, USA, FEBRUARY 24-28, 1991. BIOPHYS J.
CODEN: BIOJAU. ISSN: 0006-3495.
DOCUMENT TYPE: Conference; (Meeting)
FILE SEGMENT: BR
LANGUAGE: ENGLISH
ENTRY DATE: Entered STN: 5 May 1991
Last Updated on STN: 5 May 1991

L80 ANSWER 25 OF 29 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
ACCESSION NUMBER: 1991:179938 BIOSIS
DOCUMENT NUMBER: PREV199191094687; BA91:94687
TITLE: CRYSTALLIZATION AND PRELIMINARY **X-RAY DIFFRACTION STUDIES OF NUCLEOSIDE DIPHOSPHATE KINASE** FROM *DICTYOSTELIUM-DISCOIDEUM*.
AUTHOR(S): DUMAS C [Reprint author]; LEBRAS G; WALLET V; LACOMBE M-L; VERON M; JANIN J
CORPORATE SOURCE: LABORATOIRE BIOLOGIE PHYSICOCHIMIQUE, BAT 433 UNIVERSITE PARIS-SUD, ORSAY, FR
SOURCE: Journal of Molecular Biology, (1991) Vol. 217, No. 2, pp. 239-240.
CODEN: JMOBAK. ISSN: 0022-2836.
DOCUMENT TYPE: Article
FILE SEGMENT: BA
LANGUAGE: ENGLISH
ENTRY DATE: Entered STN: 19 Apr 1991
Last Updated on STN: 14 Jun 1991

AB Nucleoside diphosphate **kinase** from the slime mold *Dictyostelium discoideum* is highly homologous to gene products that are involved in development in *Drosophila* and in oncogenesis in human cells. The cloned protein expressed in *Escherichia coli* has been purified and crystallized in a hexagonal space group with $a = b = 74.9$.ANG., $c = 211.4$.ANG.. The asymmetric unit contains either one or two 17,000 Mr subunits of the hexamer.

L80 ANSWER 26 OF 29 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN
ACCESSION NUMBER: 1991:413452 BIOSIS
DOCUMENT NUMBER: PREV199192080417; BA92:80417

TITLE: CRYSTALLIZATION AND PRELIMINARY **X-RAY**
DIFFRACTION ANALYSIS OF **NUCLEOSIDE** DIPHOSPHATE
KINASE FROM MYXOCOCCUS-XANTHUS.

AUTHOR(S): WILLIAMS R L [Reprint author]; MUNOZ-DORADO J;
JACOBO-MOLINA A; INOUE S; INOUE M; ARNOLD E

CORPORATE SOURCE: CENTER ADVANCED BIOTECHNOL MED, DEP CHEM, RUTGERS UNIV, 679
HOES LANE, PISCATAWAY, NJ 08854-5638, USA

SOURCE: Journal of Molecular Biology, (1991) Vol. 220, No. 1, pp.
5-8.
CODEN: JMOBAK. ISSN: 0022-2836.

DOCUMENT TYPE: Article

FILE SEGMENT: BA

LANGUAGE: ENGLISH

ENTRY DATE: Entered STN: 11 Sep 1991
Last Updated on STN: 13 Nov 1991

AB **Nucleoside** diphosphate (NDP) **kinase** catalyzes the
transfer of the .gamma.-phosphate from a **nucleoside** triphosphate
to a **nucleoside** diphosphate. Human and rodent forms of this
enzyme have been shown to be suppressors of metastasis. Crystals that
diffract **X-rays** to high resolution have been obtained
for the recombinant Myxococcus xanthus NDP **kinase** expressed in
and purified from Escherichia coli. Two crystal forms have been obtained.
Both forms are orthorhombic, space group I222 (or I212121) with a = 267.1
A, b = 74.01 A and c = 75.1 A for form I and a = 53.5 A, b = 74.0 A and c
= 75.1 A for form II. Form I appears to have five molecules in the
asymmetric unit approximately related to each other by a translation of
0.2 along the a axis. Diffraction data have been recorded to 1.9 A for
form I and to 2.2 A for form II.

L80 ANSWER 27 OF 29 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: 1984:334033 BIOSIS

DOCUMENT NUMBER: PREV198478070513; BA78:70513

TITLE: CRYSTALLOGRAPHIC STUDIES OF PROTEIN NUCLEIC-ACID
INTERACTION CATABOLITE GENE ACTIVATOR PROTEIN AND THE LARGE
FRAGMENT OF DNA POLYMERASE I.

AUTHOR(S): STEITZ T A [Reprint author]; WEBER I T; OLLIS D; BRICK P

CORPORATE SOURCE: DEP MOL BIOPHYS BIOCHEM, YALE UNIV, NEW HAVEN, CONN 06511,
USA

SOURCE: Journal of Biomolecular Structure and Dynamics, (1983) Vol.
1, No. 4, pp. 1023-1038.
CODEN: JBSDD6. ISSN: 0739-1102.

DOCUMENT TYPE: Article

FILE SEGMENT: BA

LANGUAGE: ENGLISH

AB Crystals suitable for **X-ray** crystallographic
investigation were grown of several nucleic acid binding proteins and
their analysis is in progress. These include Escherichia coli catabolite
gene activator protein (CAP) and the large fragment of DNA polymerase I
(Pol I fragment). Calculation of the electrostatic charge potential of
CAP, using coordinates refined at 2.6 .ANG. resolution, suggests an
orientation for B DNA on this repressor and activator of transcription.
Both the electrostatic calculations and detailed model building suggests
that the DNA must be bent or kinked on the protein in this orientation in
order to make sufficient protein contacts. From a 3.5 .ANG. resolution
map of Pol I fragment, it was possible to obtain a preliminary trace
through the polypeptide backbone. The large fragment consists of 2
domains. The smaller domain binds **nucleoside** monophosphate at
the edge of a mostly parallel .beta.-pleated sheet, a structure that is
reminiscent of **kinase** and dehydrogenase nucleotide binding
domains. The larger domain contains .apprx. 2/3 of the fragment and is
mostly .alpha.-helical but with a least one 4-stranded antiparallel
.beta.-sheet. The **nucleoside** monophosphate binds with its 5'
phosphate on the Mg and is apparently in the conformation of nucleotides
in B DNA.

L80 ANSWER 28 OF 29 BIOSIS COPYRIGHT 2004 BIOLOGICAL ABSTRACTS INC. on STN

ACCESSION NUMBER: 1983:318017 BIOSIS

DOCUMENT NUMBER: PREV198376075509; BA76:75509

TITLE: THE COMPLETE AMINO-ACID SEQUENCE OF YEAST
SACCHAROMYCES-CEREVISIAE PHOSPHO GLYCERATE **KINASE**
EC-2.7.2.3.

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 AB The complete amino acid sequence of yeast phosphoglycerate **kinase**
 , comprising 415 residues, was determined. The sequence of residues 1-173
 was deduced mainly from nucleotide sequence analysis of a series of
 overlapping fragments derived from the relevant portion of a 2.95-kilobase
 endonuclease-HindIII-digest fragment containing the yeast phosphoglycerate
kinase gene. The sequence of residues 174-415 was deduced mainly
 from amino acid sequence analysis of 3 CNBr-cleavage fragments and from
 peptides derived from these fragments after digestion by a number of
 proteolytic enzymes. Cleavage at the 2 tryptophan residues with
 o-iodosobenzoic acid was also used to isolate fragments suitable for amino
 acid sequence analysis. Determination of the complete sequence now allows
 a detailed interpretation of the existing high-resolution **X-**
ray-crystallographic structure. The sequence -Ile-Ile-Gly-Gly-Gly-
 occurs twice in distant parts of the linear sequence (residues 232-236
 and 367-371). Both these regions contribute to the **nucleoside**
 phosphate-binding site. A comparison of the sequence of yeast
 phosphoglycerate **kinase** reported here with the sequences of
 phosphoglycerate **kinase** from horse muscle and human erythrocytes
 shows that the yeast enzyme is 64% identical with the mammalian enzymes.
 The yeast has strikingly fewer methionine, cysteine and tryptophan
 residues.

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ACCESSION NUMBER: 1974:34494 CAPLUS
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 TITLE: Enzymic synthesis and crystallographic
 characterization of an isomorphous derivative of yeast
 formylatable methionine transfer ribonucleic acid
 containing iodocytidine
 AUTHOR(S): Pasek, Mark; Venkatappa, M. P.; Sigler, Paul B.
 CORPORATE SOURCE: Dep. Biochem., Univ. Chicago, Chicago, IL, USA
 SOURCE: Biochemistry (1973), 12(24), 4834-40
 CODEN: BICHAW; ISSN: 0006-2960
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 LANGUAGE: English
 AB Isomorphous derivs. of yeast tRNA^fMet, yeast tRNA^fMet-A72-ioC-C-A (where
 ioC = iodocytidine) and yeast tRNA^fMet-A72-C-C-A were synthesized,
 crystd., and characterized by **x-ray** diffraction. The
 synthetic procedure was as follows. Yeast tRNA^fMet-A72 was prepd. by
 controlled snake venom phosphodiesterase digestion of yeast tRNA^fMet and
 the terminal trinucleotide was subsequently rebuilt with the appropriate
 radioactive **nucleoside** triphosphates and yeast
 nucleotidyltransferase. The terminal sequences were established by anal.
 of the radioactive products of a combined pancreatic RNase and
bacterial alk. phosphatase digest. Both products were
 readily aminoacylated. The crystallog. coordinates of the I atom were
 established by a 3 dimensional difference Fourier synthesis at 6 .ANG.
 using phases obtained from 3 other isomorphous derivs. The position is
 consistent with the 3-dimensional difference Patterson synthesis.

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